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Chemical Physics Letters 331–340 (2001) 1–78

CHEMICAL PHYSICS LETTERS

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Author Index to Volume 331–340

Abboud, J.-L.M., O. Castaño, J.Z. Dávalos and R. Gomperts, The standard enthalpies of formation of 1- and 2-Adamantyl cations and radicals. An ab initio study 337 (2001) 327
Abe, S., see Mukai, K. 336 (2001) 445
Abergel, D., see Louis-Joseph, A. 337 (2001) 92
Achiba, Y., see Smith, B.W. 331 (2000) 137
Achiba, Y., see Sen, R. 332 (2000) 467
Achiba, Y., see Fujiwara, A. 336 (2001) 205
Achiba, Y., see Sen, R. 340 (2001) 242
Adam, W., V. Martí, C. Sahin and A.V. Trofimov, Stereoselective formation of inverted housane in the denitrogenation of the diazenyl diradical photolytically derived from a stereolabeled diazabicyclo[2,2,1]hept-2-ene with bridgehead substituents as a function of solvent- and temperature-varied viscosity 340 (2001) 26
Adamowicz, L., see Dkhissi, A. 331 (2000) 553
Adamowicz, L., see Carles, S. 334 (2001) 374
Adamowicz, L., see Cafiero, M. 335 (2001) 404
Adu, C.K.W., G.U. Sumanasekera, B.K. Pradhan, H.E. Romero and P.C. Eklund, Carbon nanotubes: A thermoelectric nano-nose 337 (2001) 31
Agafonov, V., see Davydov, V.A. 333 (2001) 224
Agmon, N., see Popov, A.V. 340 (2001) 151
Agranovich, V.M., K. Schmidt and K. Leo, "Surface states in molecular chains with strong mixing of Frenkel and charge-transfer excitons" [Chemical Physics Letters 325 (2001) 308] 336 (2001) 536
Ågren, H., see Mochizuki, Y. 336 (2001) 451
Ågren, H., see Luo, Y. 337 (2001) 176
Ahmed, M., D.S. Peterka, P. Regan, X. Liu and A.G. Suits, Ion pair imaging spectroscopy: $CH_3Cl \rightarrow CH_3^+ + Cl^-$ 339 (2001) 203
Ahmed, N., see Khan, K.M. 339 (2001) 179
Ahn, J., see Gan, B. 333 (2001) 23
Ahner, J., see Lee, J.-G. 340 (2001) 21
Aizawa, T., see Kanakubo, M. 338 (2001) 95
Akasaka, T., see Kubozono, Y. 335 (2001) 163
Åkesson, E., see Rasmusson, M. 335 (2001) 201
Alagia, M., see Polzonetti, G. 340 (2001) 449
Alam, T.M. and D.P. Lang, Probing dissolution surface structure in phosphate glasses using $^1H^{31}P$ cross-polarization edited radio frequency dipolar recoupling experiments 336 (2001) 385
Albuquerque, R.Q., G.B. Rocha, O.L. Malta and P. Porcher, On the charge factors of the simple overlap model for the ligand field in lanthanide coordination compounds 331 (2000) 519

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PII: S0009-2614(01)00715-1

Alconcel, L.-N.S., see Li, R. 336 (2001) 81
Alexandre, M., see Mesnil, H. 338 (2001) 269
Alkorta, I., see Espinosa, E. 336 (2001) 457
Allen, M.P., Pressure tensor profiles at the isotropic–nematic interface 331 (2000) 513
Allouche, H., see Mittal, J. 339 (2001) 311
Allouchi, H., see Davydov, V.A. 333 (2001) 224
Alonso, J.A., see Pis Diez, R. 332 (2000) 481
Alonso, J.L., see Antolínez, S. 334 (2001) 250
Alparone, A., see Millefiori, S. 332 (2000) 175
Altamura, P., see Polzonetti, G. 340 (2001) 449
Alves de Carvalho, C.A., see Marques-Netto, A. 333 (2001) 371
Alzetta, G., see Bernheim, R.A. 332 (2000) 1
Amatsutsumi, S.-i., see Judai, K. 334 (2001) 277
Amo, Y. and Y. Tominaga, The Landau–Placzek ratio of water–alcohol binary mixtures 332 (2000) 521
Amon, L.M., see Miller, M.A. 331 (2000) 278
Amutha, R., V. Subramanian and B. Unni Nair, Free energy calculation for DNA bases in various solvents using Flory–Huggins theory 335 (2001) 489
Ancian, B., D. Canet and P. Mutzenhardt, Measurement of weak heteronuclear (^{13}C–^{1}H) Overhauser effects involving carbons not directly bonded to protons 336 (2001) 410
Anderson, A.J., see Mayanovic, R.A. 336 (2001) 212
Anderson, S.K., see Michael, E.A. 338 (2001) 277
Andersson, M.R., see Theander, M. 337 (2001) 277
Andrés, J., see Beltrán, A. 338 (2001) 224
Andrés, J., see Calatayud, M. 333 (2001) 493
Andrés, J., see Oliva, M. 340 (2001) 391
Andraud, C., see Schanne-Klein, M.C. 338 (2001) 159
Andraud, C., see Mesnil, H. 338 (2001) 269
Andruniow, T., M.Z. Zgierski and P.M. Kozlowski, DFT–SQM force field for cobalt corrinoids 331 (2000) 502
Andruniow, T., M.Z. Zgierski and P.M. Kozlowski, New light on the Co–C bond activation in B_{12}-dependent enzymes from density functional theory 331 (2000) 509
Andrzejak, M. and P. Petelenz, Mesoscopic disorder in thin film spectra: absorption spectroscopy of sexithiophene 332 (2000) 435
Andrzejak, M., see Munn, R.W. 336 (2001) 357
Andzelm, J., R.D. King-Smith and G. Fitzgerald, Geometry optimization of solids using delocalized internal coordinates 335 (2001) 321
Anglaret, E., see Bendiab, N. 339 (2001) 305
Ángyán, J.G., see Dehez, F. 338 (2001) 180
Anpo, M., see Furube, A. 336 (2001) 424
Antipin, S.A., A.N. Petrukhin, F.E. Gostev, V.S. Marevtsev, A.A. Titov, V.A. Barachevsky, Yu.P. Strokach and O.M. Sarkisov, Femtosecond transient absorption spectroscopy of non-substituted photochromic spirocompounds 331 (2000) 378
Antoine, R., see Dugourd, P. 336 (2001) 511
Antolínez, S., J.C. López and J.L. Alonso, Rotational spectra and structure of the hydrogen-bonded complex oxetane···HCl 334 (2001) 250
Aoki, M., see Hino, S. 337 (2001) 65
Aouni, M., see Pouchan, C. 334 (2001) 352

Arakawa, H., see Zou, Z. 332 (2000) 271
Arakawa, H., see Zou, Z. 333 (2001) 57
Araki, Y., K. Maeda and H. Murai, Observation of two-spin controlling of a radical pair by pulsed irradiation of microwave monitored by absorption detected magnetic resonance 332 (2000) 515
Arbuznikov, A.V. and M. Hendrickx, On the local structure of the correlation factor for the ground state of the helium atom 334 (2001) 325
Ardelean, I. and R. Kimmich, Erratum to "Demagnetizing field effects on the Hahn echo" [Chem. Phys. Lett. 320 (2000) 81] 332 (2000) 624
Arkhipov, V.I., E.V. Emelianova and H. Bässler, A tandem mechanism of charge-carrier photogeneration in disordered organic materials 340 (2001) 517
Armand, X., see Ténégal, F. 335 (2001) 155
Armstrong, J., L. Degoricija, A. Hildebrand, J. Koehne and P.E. Fleming, The ionization energies of the isomers of CN_2 332 (2000) 591
Arthurs, S., see Verkhivker, G.M. 336 (2001) 495
Arthurs, S., see Verkhivker, G.M. 337 (2001) 181
Asahi, T., see Furube, A. 336 (2001) 424
Asano, T., see Yoshida, N. 332 (2000) 265
Ascenzi, D., see Rudić, S. 332 (2000) 487
Ashbrook, S.E. and S. Wimperis, Novel two-dimensional NMR methods that combine single-quantum cross-polarization and multiple-quantum MAS of quadrupolar nuclei 340 (2001) 500
Asplund, M.C., M. Lim and R.M. Hochstrasser, Erratum to: "Spectrally resolved three pulse photon echoes in the vibrational infrared" [Chem. Phys. Lett. 323 (2001) 269–277] 340 (2001) 611
Assenmacher, W., see Möschel, C. 335 (2001) 9
Åstrand, P.-O., see Ruud, K. 337 (2001) 217
Ataka, K., see Dreesen, L. 333 (2001) 327
Ataka, M., see Tachibana, M. 332 (2000) 259
Athayde-Filho, P.A.F., see Rakov, N. 332 (2000) 13
Attinà, M., see Cacace, F. 339 (2001) 71
Ausmees, A., see Hjelte, I. 334 (2001) 151
Azoulay, J., A. Débarre, A. Richard, P. Tchénio, S. Bandow and S. Iijima, Polarised Raman spectroscopy on a single class of single-wall nanotubes by nano surface-enhanced scattering 331 (2000) 347

Babu, Y., see Bhide, M.K. 332 (2000) 98
Bacalis, N.C., Comment on the formation of $He_2^{-4}I_g$ states 331 (2000) 323
Bacchiocchi, C., M. Brunelli and C. Zannoni, Energy transfer and orientational dynamics in isotropic and nematic phases. A computer simulation approach 336 (2001) 253
Bae, S.Y., H. Yang and J. Park, The steric hindrance of methyl groups in collisional quenching of highly vibrationally excited methyl-substituted pyrazines by He, Ar, and Kr 336 (2001) 219
Baeck, K.K. and Y. Joo, The potential energy surface of excited singlet states of BCl by using the equation-of-motion coupled-cluster theory 337 (2001) 190
Baer, M. and R. Englman, Electronic non-adiabatic transitions: the line integral and approximations 335 (2001) 85
Baer, M., see Mebel, A.M. 336 (2001) 135

Bagryanskaya, E.G., see Fedin, M.V. 339 (2001) 395
Bagus, P.S., see Wöll, Ch. 332 (2000) 553
Bai, C., see Wang, X. 339 (2001) 36
Bakes, E.L.O., see Walch, S.P. 333 (2001) 6
Balakrishnan, N., see Ramachandran, B. 332 (2000) 562
Balfour, W.J., see Ding, C.-F. 331 (2000) 163
Ballester, P., see Quiñonero, D. 339 (2001) 369
Bando, Y., see Ma, R. 337 (2001) 61
Bandow, S., M. Takizawa, K. Hirahara, M. Yudasaka and S. Iijima, Raman scattering study of double-wall carbon nanotubes derived from the chains of fullerenes in single-wall carbon nanotubes 337 (2001) 48
Bandow, S., see Azoulay, J. 331 (2000) 347
Bandrauk, A.D. and S. Chelkowski, On laser coulomb explosion imaging of proton motion 336 (2001) 518
Barachevsky, V.A., see Antipin, S.A. 331 (2000) 378
Baranek, Ph., A. Lichanot, R. Orlando and R. Dovesi, Structural and vibrational properties of solid $Mg(OH)_2$ and $Ca(OH)_2$ – performances of various hamiltonians 340 (2001) 362
Bardhan, S., see Gandy, P.J.F. 336 (2001) 187
Barnes, M.D., see Gray, S.K. 333 (2001) 308
Baronavski, A.P. and J.C. Owrutsky, Ketone excited state lifetimes measured by deep UV ultrafast photoionization spectroscopy 333 (2001) 36
Barone, V., see di Matteo, A. 335 (2001) 427
Barone, V., see Improta, R. 336 (2001) 349
Barrientos, C., see Redondo, P. 335 (2001) 64
Barrios, R., see Skurski, P. 337 (2001) 143
Barros, W., see Hallwass, F. 335 (2001) 43
Barry, H.R., L. Corner, G. Hancock, R. Peverall and G.A.D. Ritchie, Cavity-enhanced absorption spectroscopy of methane at 1.73 μm 333 (2001) 285
Bartels, C., Analyzing biased Monte Carlo and molecular dynamics simulations 331 (2000) 446
Bartlett, R.J., see Henderson, T.M. 337 (2001) 138
Bassett, W.A., see Mayanovic, R.A. 336 (2001) 212
Bässler, H., see Meskers, S.C.J. 339 (2001) 223
Bässler, H., see Arkhipov, V.I. 340 (2001) 517
Bässler, M., see Hjelte, I. 334 (2001) 151
Batlogg, B., see Frolov, S.V. 334 (2001) 65
Baudin, M., M. Wojcik, K. Hermansson, A.E.C. Palmqvist and M. Muhammed, MD simulations of a doped ceria surface – very large surface ion motion 335 (2001) 517
Baumgärtel, H., see Seccombe, D.P. 339 (2001) 405
Bauschlicher, C.W. and C.R. So, Using hydrogen and chlorine on Si(1 1 1) to store data 333 (2001) 1
Bauschlicher, C.W., see Walch, S.P. 333 (2001) 6
Bawagan, A.D.O., The calculation and measurement of synchrotron radiation flux: finite emittance effects 334 (2001) 187
Bazalgette Courrèges-Lacoste, G., J.P. Sprengers, J. Bulthuis, S. Stolte, T. Motylewski and H. Linnartz, Vibrationally excited state spectroscopy of radicals in a supersonic plasma 335 (2001) 209
Bazan, G.C., see Wang, S. 333 (2001) 437
Bazeia, D., V.B.P. Leite, B.H.B. Lima and F. Moraes, Soliton model for proton conductivity in Langmuir films 340 (2001) 205

Becerra, R., I.W. Carpenter, G.J. Gutsche, K.D. King, W.D. Lawrance, W.S. Staker and R. Walsh, The gas-phase reaction of SiH_2 with dimethylether: kinetic evidence for direct formation of a donor–acceptor adduct 333 (2001) 83
Becker, A., see Muth-Böhm, J. 337 (2001) 313
Becker, I., see Weber, J.M. 339 (2001) 337
Becker, J.A., see Rosemeyer, M. 339 (2001) 323
Becucci, M., see Pietraperzia, G. 335 (2001) 195
Bedrov, D., see Borodin, O. 336 (2001) 292
Bégué, D., see Mérawa, M. 334 (2001) 403
Bégué, D., see Pouchan, C. 334 (2001) 352
Béguin, F., see Bendiab, N. 339 (2001) 305
Belau, L. and Y. Haas, The nature of the exalted Kekulé vibration of styrene and other benzene derivatives in the S_1 state 333 (2001) 297
Belchior, J.C. and J.P. Braga, Calculation of three dimensional cross-sections for the Ar–N_2 system from two-dimensional coupled equations plus a three-dimensional boundary condition 332 (2000) 159
Bell, R.L., see Borodin, O. 336 (2001) 292
Bellert, D. and W.H. Breckenridge, A resonant two-color photoionization threshold determination of the ionization energy of the LiOLi molecule 337 (2001) 103
Bello, I., see Zhou, X.T. 332 (2000) 215
Beltrán, A., J. Andrés, M. Calatayud and J.B.L. Martins, Theoretical study of ZnO (1 0 $\bar{1}$ 0) and Cu/ZnO (1 0 $\bar{1}$ 0) surfaces 338 (2001) 224
Beltrán, A., see Calatayud, M. 333 (2001) 493
Benco, L., D. Tunega, J. Hafner and H. Lischka, Ab initio density functional theory applied to the structure and proton dynamics of clays 333 (2001) 479
Bendiab, N., A. Righi, E. Anglaret, J.L. Sauvajol, L. Duclaux and F. Béguin, Low-frequency Raman modes in Cs- and Rb-doped single wall carbon nanotubes 339 (2001) 305
Bendix, J., see Spichiger, D. 337 (2001) 391
Benny Gerber, R., see Lundell, J. 331 (2000) 308
Bensasson, R.V., see Kordatos, K. 334 (2001) 221
Bensasson, R.V., see Schwell, M. 339 (2001) 29
Bentley, J., B.J. Cotterell, A. Langham and R.J. Stickland, 2+1 resonance-enhanced multiphoton ionisation spectroscopy of the high v_2 levels of the $\tilde{B}^1E''$ Rydberg state of $NH_3(ND_3)$ 332 (2000) 85
Berardi, R., see Burnell, E.E. 331 (2000) 455
Berberan-Santos, M.N., see Bodunov, E.N. 340 (2001) 137
Berden, G., see Peeters, R. 337 (2001) 231
Berezhkovskii, A.M., M. Boguñá and G.H. Weiss, Evaluation of rate constants for conformational transitions using single-molecule fluorescence spectroscopy 336 (2001) 321
Berg, L.-E., see Derkatch, A. 332 (2000) 278
Berg, L.-E., see Zhang, B. 339 (2001) 438
Bernhardt, T.M., see Socaciu, L.D. 340 (2001) 282
Bernheim, R.A., J.H. Xu, F. Mango and G. Alzetta, Threshold energy for the photon-stimulated desorption of Rb atoms from polydimethylsiloxane films 332 (2000) 1
Bernier, P., see Stepanek, I. 331 (2000) 125
Berski, S., see Mierzwicki, K. 331 (2000) 538
Bertran, J., see Rodríguez-Santiago, L. 334 (2001) 112
Besemann, D.M., see Murdoch, K.M. 335 (2001) 349

Bettinger, H.F. and G.E. Scuseria, The infrared vibrational spectra of the two major C_{84} isomers 332 (2000) 35
Bevan, J.W., see McIntosh, A. 331 (2000) 95
Bhanuprakash, K., see Vivekananda, S. 332 (2000) 251
Bhide, M.K., R.M. Kadam, Y. Babu, V. Natarajan and M.D. Sastry, EPR and ENDOR studies of self(α)-irradiation effects in Pu(VI) oxalate: evidence for participation of 5f electrons of ^{239}Pu in chemical bonding with CO_2^- 332 (2000) 98
Bielschowsky, C.E., see Rocha, A.B. 337 (2001) 331
Bieske, E.J., see Wild, D.A. 332 (2000) 531
Billeter, S.R., see Iordanov, T. 338 (2001) 389
Billing, G.D., A split-Lanczos method for solving time-dependent discrete variable Gauss–Hermite dynamics 339 (2001) 237
Billing, G.D., see Rutigliano, M. 340 (2001) 13
Binning Jr. R.C., see Ishikawa, Y. 338 (2001) 353
Birczyński, A., Z.T. Lalowicz, Z. Olejniczak, G. Stoch and B. Petelenz, Low temperature domain structure in $(ND_4)_2TeCl_6$ detected by deuteron NMR spectroscopy 339 (2001) 229
Birkett, P.R., see Rice, J.H. 335 (2001) 553
Bishop, A.R., see Tretiak, S. 331 (2000) 561
Bittererová, M., see Schinke, R. 332 (2000) 611
Bittererová, M., T. Brinck and H. Östmark, Theoretical study of the singlet electronically excited states of N_4 340 (2001) 597
Bitzer, T., T. Dittrich, T. Rada and N.V. Richardson, The electronic properties at the maleic anhydride/Si(100)-2 × 1 interface 331 (2000) 433
Björneholm, O., see Hjelte, I. 334 (2001) 151
Blanco, F., see García, G. 335 (2001) 227
Bobbert, P.A., see van der Horst, J.-W. 334 (2001) 303
Bodunov, E.N., M.N. Berberan-Santos and J.M.G. Martinho, Dynamics of electronic energy transfer in linear chain polymers 340 (2001) 137
Boens, N., see Novikov, E. 338 (2001) 151
Boguñá, M., see Berezhkovskii, A.M. 336 (2001) 321
Böhm, M.C., J. Schulte and R. Ramírez, Nuclear quantum effects in calculated NMR shieldings of ethylene; a Feynman path integral – ab initio study 332 (2000) 117
Bondo Pedersen, T., B. Fernández and H. Koch, Comment on "The importance of high-order correlation effects for the CO–CO interaction potential" [Chem. Phys. Lett. 314 (1999) 326] 334 (2001) 419
Bonnet, L. and J.C. Rayez, Kinematic rotations in RRKM theory 338 (2001) 385
Bordat, P. and R. Brown, Elucidation of optical switching of single guest molecules in terrylene/*p*-terphenyl mixed crystals 331 (2000) 439
Borges, I., see Varandas, A.J.C. 331 (2000) 285
Borissevitch, G.P., see Haas, H. 335 (2001) 510
Borodin, O., R.L. Bell, Y. Li, D. Bedrov and G.D. Smith, Polarizable and nonpolarizable potentials for K^+ cation in water 336 (2001) 292
Borovykh, I.V., L.V. Kulik, S.A. Dzuba and A.J. Hoff, Selective excitation in pulsed EPR of spin-correlated radical pairs: electron–electron interactions, zero-, single-, and double-quantum relaxation and spectral diffusion 338 (2001) 173
Borowski, T., see Brocławik, E. 339 (2001) 433
Borst, D.R., see Hockridge, M.R. 334 (2001) 31

Boudon, V., see Rotger, M. 339 (2001) 83
Boul, P.J., see Walters, D.A. 338 (2001) 14
Boulet, A.M., E.D. Walter, D.A. Schwartz, G.J. Gerfen, P.R. Callis and D.J. Singel, Electronic structure and hyperfine interactions in thioether-substituted tyrosyl radicals 331 (2000) 108
Bourhill, G., L.O. Pålsson, I.D.W. Samuel, I.C. Sage, I.D.H. Oswald and J.P. Duignan, The solid-state photoluminescent quantum yield of triboluminescent materials 336 (2001) 234
Bourhill, G., see Goedert, R.V. 332 (2000) 225
Boustani, I., see Shen, Z. 339 (2001) 362
Boutreau, L., E. Leon, A. Luna, P. Toulhoat and J. Tortajada, Reactions between small organic molecules and Ag^+ in the gas-phase. A theoretical study 338 (2001) 74
Bouzida, D., see Verkhivker, G.M. 336 (2001) 495
Bouzida, D., see Verkhivker, G.M. 337 (2001) 181
Bowman, J.M., see Zou, S. 339 (2001) 290
Brabec, C.J., G. Zerza, G. Cerullo, S. De Silvestri, S. Luzzati, J.C. Hummelen and S. Sariciftci, Tracing photoinduced electron transfer process in conjugated polymer/fullerene bulk heterojunctions in real time 340 (2001) 232
Brabec, C.J., see Miller, E.K. 335 (2001) 23
Bradley, D.D.C., see Buckley, A.R. 339 (2001) 331
Bradley, D.D.C., see Cerullo, G. 335 (2001) 27
Bradshaw, A.M., see Meißen, F. 336 (2001) 181
Braga, J.P., see Belchior, J.C. 332 (2000) 159
Braga, J.P., see Rolim, F. 332 (2000) 139
Bramwell, M.J., D.M. Rogers, J.J.W. McDouall and J.C. Whitehead, A theoretical and experimental study of the HPCl radical: the $\tilde{A}^2A' \rightarrow \tilde{X}^2A''$ visible emission spectrum 331 (2000) 483
Bräsicke, K., see Saenger, W. 336 (2001) 504
Bréchignac, C., Ph. Cahuzac, B. Concina, J. Leygnier, B. Villard, P. Parneix and Ph. Bréchignac, Experimental evidence for anharmonic and rotational effects in the evaporation of sodium clusters 335 (2001) 34
Bréchignac, Ph., see Bréchignac, C. 335 (2001) 34
Bréchignac, Ph., see Gée, Ch. 338 (2001) 130
Bréchignac, Ph., see Pino, T. 339 (2001) 64
Breckenridge, W.H., see Bellert, D. 337 (2001) 103
Brede, O., see Ganapathi, M.R. 337 (2001) 335
Brenner, D.W., see Frankland, S.J.V. 334 (2001) 18
Brenner, V., see Çarçabal, P. 336 (2001) 335
Brickmann, J., see Zahn, D. 331 (2000) 224
Briggman, K.A., P.C. Stair and E. Weitz, Surface residence time measurements of transient methyl radicals 334 (2001) 1
Brinck, T., see Bittererová, M. 340 (2001) 597
Brito, H.F., see Marques-Netto, A. 333 (2001) 371
Brocławik, E., J. Haber and W. Piskorz, Molecular mechanism of C–H bond cleavage at transition metal oxide clusters 333 (2001) 332
Brocławik, E. and T. Borowski, Time-dependent DFT study on electronic states of vanadium and molybdenum oxide molecules 339 (2001) 433
Brocklehurst, B., Effects of very strong magnetic fields on radical reactions: the role of *g*-value anisotropy. 339 (2001) 421

Brocklehurst, B., see Timmel, C.R. 334 (2001) 387
Brocks, G., see van der Horst, J.-W. 334 (2001) 303
Bródka, A., see Gwóźdź, E. 335 (2001) 71
Bromley, S.T., G. Sankar, C.R.A. Catlow, Th. Maschmeyer, B.F.G. Johnson and J.M. Thomas, New insights into the structure of supported bimetallic nanocluster catalysts prepared from carbonylated precursors: a combined density functional theory and EXAFS study 340 (2001) 524
Brotin, T., see Schanne-Klein, M.C. 338 (2001) 159
Brown, R., see Bordat, P. 331 (2000) 439
Broyer, M., see Dugourd, P. 336 (2001) 511
Brugh, D.J., see McIntosh, A. 331 (2000) 95
Brunelli, M., see Bacchiocchi, C. 336 (2001) 253
Bryant, R.G., see Korb, J.-P. 339 (2001) 77
Bu, Y., Theoretical prediction of the state–state correlation among doublet state AlSO isomers 338 (2001) 142
Bu, Y., see Feng, S. 339 (2001) 103
Buchachenko, A.A., see Krems, R.V. 335 (2001) 273
Buchachenko, A.L., F.I. Dalidchik and B.R. Shub, Single spin ESR 340 (2001) 103
Buckingham, A.D., see Champagne, B. 331 (2000) 83
Buckley, A.R., M.D. Rahn, J. Hill, J. Cabanillas-Gonzalez, A.M. Fox and D.D.C. Bradley, Energy transfer dynamics in polyfluorene-based polymer blends 339 (2001) 331
Bulthuis, J., see Bazalgette Courrèges-Lacoste, G. 335 (2001) 209
Burcl, R., see Torday, L.L. 334 (2001) 381
Bürger, H., see Rotger, M. 339 (2001) 83
Burhanudin, Z. and P. Etchegoin, Monitoring surface molecular order in discotic liquid crystals 336 (2001) 7
Burnell, E.E., C.A. de Lange and S. Gaemers, Pressure-induced change in orientational order of solutes in liquid crystals 337 (2001) 248
Burnell, E.E., R. Berardi, R.T. Syvitski and C. Zannoni, Monte Carlo simulations of zero electric field gradient liquid crystal mixtures 331 (2000) 455
Burrows, H.D., see Monkman, A.P. 340 (2001) 467
Bursill, L.A., see Prawer, S. 332 (2000) 93
Burt, S.K., see Rashin, A.A. 335 (2001) 327
Butenko, Yu. V., see Kuznetsov, V.L. 336 (2001) 397

Cabanillas-Gonzalez, J., see Buckley, A.R. 339 (2001) 331
Cacace, F., M. Attinà, A. Cartoni and F. Pepi, Gas-phase fluorination of acetylene by XeF^+: Formation, structure and reactivity of $C_2H_2F^+$ isomeric ions 339 (2001) 71
Cacciatore, M., see Rutigliano, M. 340 (2001) 13
Caetano, W., see Haas, H. 335 (2001) 510
Cafiero, M. and L. Adamowicz, Simultaneous optimization of molecular geometry and the wave function in a basis of Singer's *n*-electron explicitly correlated Gaussians 335 (2001) 404
Cahuzac, Ph., see Bréchignac, C. 335 (2001) 34
Cai, S., see Shi, Z. 336 (2001) 19
Calatayud, M., B. Silvi, J. Andrés and A. Beltrán, A theoretical study on the structure, energetics and bonding of VO_x^+ and VO_x (x=1–4) systems 333 (2001) 493
Calatayud, M., see Beltrán, A. 338 (2001) 224
Callis, P.R., see Boulet, A.M. 331 (2000) 108

Cané, E., A. Miani and A. Trombetti, The harmonic vibrational frequencies and the geometry of the $^{12}C_6H_6$ 340 (2001) 356
Canet, D., see Ancian, B. 336 (2001) 410
Canuto, S., see Rocha, W.R. 335 (2001) 127
Cao, A., L. Ci, D. Li, B. Wei, C. Xu, J. Liang and D. Wu, Vertical aligned carbon nanotubes grown on Au film and reduction of threshold field in field emission 335 (2001) 150
Cao, X.W., see Wang, Y.F. 336 (2001) 47
Cao, Y., see Shi, Z. 336 (2001) 19
Cao, Y., see Wang, Z.H. 338 (2001) 7
Capitelli, M., see Hassouni, K. 340 (2001) 322
Caprioli, R., see Resmi, M.R. 333 (2001) 515
Çarçabal, P., V. Brenner, N. Halberstadt and P. Millié, Ab initio anharmonic intermolecular potential of the C_2H_2–HCl hydrogen bonded complex 336 (2001) 335
Cardenas, G., see Lima, C.A.S. 332 (2000) 428
Caridade, P.J.S.B., see Varandas, A.J.C. 331 (2000) 331
Caridade, P.J.S.B., see Varandas, A.J.C. 339 (2001) 1
Carles, S., C. Desfrançois, J.P. Schermann, A.F. Jalbout and L. Adamowicz, Dipole-bound anion of 1,3-butanediol. Ab initio and Rydberg electron transfer spectroscopy study 334 (2001) 374
Carpenter, I.W., see Becerra, R. 333 (2001) 83
Carrapa, R.T., see Lourenço, J.M.C. 336 (2001) 431
Carravetta, V., see Polzonetti, G. 340 (2001) 449
Carter, R.T., see Li, Q. 334 (2001) 39
Carter, R.T., see Nagai, H. 331 (2000) 425
Carter, S., see Taketsugu, T. 340 (2001) 385
Cartoni, A., see Cacace, F. 339 (2001) 71
Carvalho, C.F., see Marques-Netto, A. 333 (2001) 371
Carver, G., see Spichiger, D. 337 (2001) 391
Casavant, M.J., see Walters, D.A. 338 (2001) 14
Casieri, C., A. Knijn, F. Podo and F. De Luca, ^{1}H NMR detection of ^{13}C–^{1}H bonds by double ^{13}C editing: application to the discrimination of glucose metabolites 338 (2001) 137
Castaño, F., see Redondo, C. 331 (2000) 365
Castaño, O., see Abboud, J.-L.M. 337 (2001) 327
Castellucci, E., see Pietraperzia, G. 335 (2001) 195
Catlow, C.R.A., see Bromley, S.T. 340 (2001) 524
Cavalli, A., P. Dynarowicz-Łaçtka, O.N. Oliveira Jr and E. Feitosa, Using an effective surface charge to explain surface potentials of Langmuir monolayers from dialkyldimethylammonium halides with the Gouy–Chapman theory 338 (2001) 88
Cavalli, A., see Dynarowicz-atka, P. 337 (2001) 11
Ceballos, A., see Rodriguez, A. 333 (2001) 471
Ceccherini, S. and M. Moraldi, Interatomic potentials of group IIB atoms (ground state) 337 (2001) 386
Cedeño, D.L., see Lewis, E.K. 334 (2001) 357
Cederbaum, L.S., see Dobrodey, N.V. 339 (2001) 263
Cederbaum, L.S., see Worth, G.A. 338 (2001) 219
Céolin, R., see Davydov, V.A. 333 (2001) 224
Cerofolini, G.F. and N. Re, A topological analysis of charge density in complexes between derivatives of squaric acid and ammonium cation 339 (2001) 375

Cerofolini, G.F. and N. Re, Core electrons as probes of the net-charge distribution in molecules: a case study 333 (2001) 181
Cerullo, G., S. Stagira, M. Zavelani-Rossi, S. De Silvestri, T. Virgili, D.G. Lidzey and D.D.C. Bradley, Ultrafast Förster transfer dynamics in tetraphenylporphyrin doped poly(9,9-dioctylfluorene) 335 (2001) 27
Cerullo, G., see Brabec, C.J. 340 (2001) 232
Chaban, G.M., see Lundell, J. 331 (2000) 308
Chakravorti, S., see Panja, S. 336 (2001) 57
Chakravorti, S., see Panja, S. 338 (2001) 217
Chambaud, G., see Léonard, C. 335 (2001) 97
Champagne, B., P. Fischer and A.D. Buckingham, Ab initio investigation of the sum-frequency hyperpolarizability of small chiral molecules 331 (2000) 83
Champion, P.M., see Rosca, F. 337 (2001) 107
Chan, J.C.C., C-REDOR: rotational echo double resonance under very fast magic-angle spinning 335 (2001) 289
Chandra, A.K. and T. Uchimaru, The C–H bond dissociation enthalpies of haloethers and its correlation with the activation energies for hydrogen abstraction by OH radical: A DFT study 334 (2001) 200
Chandrasekhar, J., see Puranik, M. 337 (2001) 224
Chang, C.F., see Chen, J.M. 337 (2001) 85
Chang, D.E., L.M.K. Vandersypen and M. Steffen, NMR implementation of a building block for scalable quantum computation 338 (2001) 337
Changenet-Barret, P., P. Plaza and M.M. Martin, Primary events in the photoactive yellow protein chromophore in solution 336 (2001) 439
Chao, S.D. and R.T. Skodje, The search for resonance signatures in H + D_2 reaction dynamics 336 (2001) 364
Chaplin, M.F., see Manos, G. 335 (2001) 77
Chapman, W.G., see Duda, Y. 339 (2001) 89
Chastaing, D., S.D. Le Picard, I.R. Sims, I.W.M. Smith, W.D. Geppert, C. Naulin and M. Costes, Rate coefficients and cross-sections for the reactions of $C(^3P_J)$ atoms with methylacetylene and allene 331 (2000) 170
Chattopadhyay, S., see Sett, P. 331 (2000) 215
Chau, F.-T., see Lee, E.P.F. 340 (2001) 348
Chau, P.-L., Process and thermodynamics of ligand–receptor interaction studied using a novel simulation method 334 (2001) 343
Che, C.-M., see Cheng, Y.F. 338 (2001) 308
Cheah, K.W., see Meng, J.X. 332 (2000) 313
Chelkowski, S., see Bandrauk, A.D. 336 (2001) 518
Chelmick, T., see Dickinson, H. 338 (2001) 37
Chen, C., see Gao, Y. 339 (2001) 209
Chen, D.-M., see He, T.-J. 332 (2000) 545
Chen, G., see Yokojima, S. 333 (2001) 397
Chen, H., Y. Li and A.S.-C. Cheung, Laser spectroscopy of the $B^2\Sigma^+$–$X^2\Sigma^+$ transition of TiN 335 (2001) 388
Chen, H.-Y. and W.-S. Sheu, Iodine effect on the relaxation pathway of photoexcited $I^-(H_2O)_n$ clusters 335 (2001) 475
Chen, I.-C., see Chen, S.-H. 333 (2001) 365
Chen, J., see Zhang, X.X. 333 (2001) 509

Chen, J.M., P. Nachimuthu, J.Y. Lin, I.P. Hong, C.F. Chang and H.D. Yang, Origin of size effect on superconductivity in ($R_{0.8}$ $Pr_{0.2}$) $Ba_2Cu_3O_7$ studied by soft X-ray absorption spectroscopy 337 (2001) 85
Chen, K.-m., Angular momentum coupling in triatomic pre-dissociations 333 (2001) 119
Chen, L.X., see He, J.L. 340 (2001) 431
Chen, L.X., see Manas, E.S. 331 (2000) 299
Chen, M.-D., B.-Y. Tang, K.-L. Han and N.-Q. Lou, Quasi-classical trajectory study of the DCl/HCl product branching ratios for the Cl + HD reaction on BW2 potential energy surface 337 (2001) 349
Chen, R., K.-C. Zhang, L. Liu, X.-S. Li and Q.-X. Guo, Substituent effects in X—C≡C—H···NH_3 (or OH_2, FH) hydrogen bonding 338 (2001) 61
Chen, R.J., see Zhang, Y. 331 (2000) 35
Chen, S.A., see White, J.D. 338 (2001) 263
Chen, S.-H., L.-K. Chu, Y.-J. Chen, I.-C. Chen and Y.-P. Lee, Detection of ClCO with time-resolved Fourier-transform infrared absorption spectroscopy 333 (2001) 365
Chen, T., see Heid, M. 334 (2001) 119
Chen, X., see Fang, L. 332 (2000) 299
Chen, X., see Han, J. 332 (2000) 243
Chen, X.H., F.M. Deng, J.X. Wang, H.S. Yang, G.T. Wu, X.B. Zhang, J.C. Peng and W.Z. Li, New method of carbon onion growth by radio-frequency plasma-enhanced chemical vapor deposition 336 (2001) 201
Chen, Y. and M.R. Topp, Conformational barrier crossing in the water dimer cluster of coumarin 151 studied by infrared–optical double-resonance spectroscopy 337 (2001) 284
Chen, Y., see Gao, Y. 339 (2001) 209
Chen, Y.-C., see Chou, P.-T. 340 (2001) 89
Chen, Y.-J., P.T. Fenn and C.Y. Ng, Direct identification of product CH_2SH^+/CH_3S^+ structures in the dissociation of $CH_3CH_2SH^+$ and $CH_3SCH_3^+$ via collisional activation 336 (2001) 105
Chen, Y.-J., see Chen, S.-H. 333 (2001) 365
Chen, Z., G. Lin and J. Zhong, Diffusion of intermolecular zero- and double-quantum coherences in two-component spin systems 333 (2001) 96
Chen, Z., see Chen, Z. 333 (2001) 126
Chen, Z., see Lin, G. 335 (2001) 249
Chen, Z., Z. Chen and J. Zhong, Quantitative study of longitudinal relaxation related to intermolecular dipolar interactions in solution NMR 333 (2001) 126
Cheng, J., S. Wang, X.-Y. Li, Y. Yan, S. Yang, C.L. Yang, J.N. Wang and W.K. Ge, Fast interfacial charge separation in chemically hybridized CdS-PVK nanocomposites studied by photoluminescence and photoconductivity measurements 333 (2001) 375
Cheng, L.F., see Liao, L.S. 333 (2001) 212
Cheng, Y.F., D.L. Phillips, G.Z. He, C.-M. Che and Y. Chi, Resonance Raman and density functional study of the A-band absorption of $C_5H_5[WC{\equiv}CPh]O_2$ 338 (2001) 308
Cheng, Y.-M., see Chou, P.-T. 340 (2001) 89
Cheshnovsky, O., see Weber, J.M. 339 (2001) 337
Cheskis, S., see Lozovsky, V.A. 332 (2000) 508
Cheung, A.S.-C., see Chen, H. 335 (2001) 388
Cheung, A.S-C., see Shi, Q. 339 (2001) 154
Chew, K., see Gan, B. 333 (2001) 23
Chi, Y., see Cheng, Y.F. 338 (2001) 308

Chie, K., N. Okazaki, Y. Tanimoto and I. Hanazaki, Tristability in the bromate–sulfite–hydrogencarbonate pH oscillator 334 (2001) 55
Chin, S.L., see Muth-Böhm, J. 337 (2001) 313
Chipot, C. and F.J. Luque, Fast evaluation of induction energies: a second-order perturbation theory approach 332 (2000) 190
Chipot, C., see Dehez, F. 338 (2001) 180
Chomiak, D., see Taleb-Bendiab, A. 334 (2001) 195
Chosrowjan, H., see Kandori, H. 334 (2001) 271
Chou, I.-M., see Mayanovic, R.A. 336 (2001) 212
Chou, P.-T., Y.-C. Chen, W.-S. Yu and Y.-M. Cheng, Spectroscopy and dynamics of excited-state intramolecular proton-transfer reaction in 5-hydroxyflavone 340 (2001) 89
Chu, L.-K., see Chen, S.-H. 333 (2001) 365
Chu, S.-Y., see Lin, C.-L. 339 (2001) 147
Chua, S.J., see Guo, Y.P. 339 (2001) 319
Chung, G. and Y. Kwon, Molecular structures of gauche and anti conformers for oxalyl bromide: ab initio and DFT calculations 333 (2001) 189
Churikov, V.M., M.-F. Hung, C.-C. Hsu, C.-W. Shiau and T.-Y. Luh, Encoding of macroscopic second-order non-linearity via all-optical polar alignment in substituted norbornene polymer thin films 332 (2000) 19
Chuvilin, A.L., see Kuznetsov, V.L. 336 (2001) 397
Ci, L., see Cao, A. 335 (2001) 150
Cintolesi, F., see Timmel, C.R. 334 (2001) 387
Cioslowski, J., G. Liu and R.A. Mosquera Castro, Badger's rule revisited 331 (2000) 497
Claes, L., J.-P. François and M.S. Deleuze, Molecular packing of oligomer chains of poly(p-phenylene vinylene) 339 (2001) 216
Clark, J., M. Konopka, L.-M. Zhang and E.R. Grant, The $A^1\Pi$–$X^1\Sigma^+$ (2,0) transition in ^{11}BH and ^{10}BH observed by (1 + 2)-photon resonance-enhanced multiphoton ionization spectroscopy 340 (2001) 45
Clary, D.C., see van Mourik, T. 331 (2000) 253
Claye, A., S. Rahman, J.E. Fischer, A. Sirenko, G.U. Sumanasekera and P.C. Eklund, In situ Raman scattering studies of alkali-doped single wall carbon nanotubes 333 (2001) 16
Cleaver, D.J. and P.I.C. Teixeira, Discontinuous structural transition in a thin hybrid liquid crystal film 338 (2001) 1
Clements, A.F., see Goedert, R.V. 332 (2000) 225
Clemmer, D.E., see Ideue, S. 337 (2001) 79
Colbert, D.T., see Walters, D.A. 338 (2001) 14
Cole, M.W., see Kostov, M.K. 332 (2000) 26
Collera, O., see García-Jiménez, F. 331 (2000) 42
Collet, A., see Schanne-Klein, M.C. 338 (2001) 159
Collins, M.A., see Song, K. 335 (2001) 481
Colson, A.B., see Verkhivker, G.M. 336 (2001) 495
Colson, A.B., see Verkhivker, G.M. 337 (2001) 181
Compagnon, I., see Dugourd, P. 336 (2001) 511
Compton, R.N., see Hinde, R.J. 339 (2001) 167
Concina, B., see Bréchignac, C. 335 (2001) 34
Condon, N.J., see Murdoch, K.M. 335 (2001) 349
Cong, S., see Sun, M. 339 (2001) 413
Continetti, R.E., see Li, R. 336 (2001) 81

Corner, L., see Barry, H.R. 333 (2001) 285
Cory, D.G., see Leu, G. 332 (2000) 344
Costa, A., see Quiñonero, D. 339 (2001) 369
Costes, M., see Chastaing, D. 331 (2000) 170
Costes, M., see Geppert, W.D. 333 (2001) 51
Cotlet, M., J. Hofkens, F. Köhn, J. Michiels, G. Dirix, M. Van Guyse, J. Vanderleyden and F.C. De Schryver, Collective effects in individual oligomers of the red fluorescent coral protein DsRed 336 (2001) 415
Cotlet, M., see Hofkens, J. 333 (2001) 255
Cotterell, B.J., see Bentley, J. 332 (2000) 85
Couris, S., see Juha, L. 335 (2001) 539
Couris, S., see Koudoumas, E. 335 (2001) 533
Cours, T., P. Rosmus and V.G. Tyuterev, Ab initio dipole moment function of H_2S 331 (2000) 317
Coutinho, K., see Rocha, W.R. 335 (2001) 127
Crépin, C., see Gée, Ch. 338 (2001) 130
Cremer, D., E. Kraka and C. Sosa, First evidence for the production of OH radicals by carbonyl oxides in solution phase – A DFT investigation 337 (2001) 199
Cristina dos Santos, M., see Dynarowicz-atka, P. 337 (2001) 11
Cross, J.B. and H.B. Schlegel, Molecular orbital studies of titanium nitride chemical vapor deposition: gas phase β-elimination 340 (2001) 343
Cruse, H.A., see Monti, O.L.A. 333 (2001) 146
Császár, P., see Torday, L.L. 334 (2001) 381
Csizmadia, I.G., see Torday, L.L. 334 (2001) 381
Curl, R.F., see Sun, F. 337 (2001) 72
Czuchaj, E. and M. Krośnicki, CCSD(T) calculation of the ground-state potential curves for the Zn-rare gas van der Waals molecules 335 (2001) 440

da Rocha, G.B., see Rakov, N. 332 (2000) 13
Dai, H., see Zhang, Y. 331 (2000) 35
Dai, Z., see Yang, X. 334 (2001) 257
Dalgarno, A., see Ramachandran, B. 332 (2000) 562
Dalidchik, F.I., see Buchachenko, A.L. 340 (2001) 103
Dalton, L.R., see Pereverzev, Y.V. 340 (2001) 328
Dalton, L.R., see Strohkendl, F.P. 331 (2000) 354
Daly, G.M., D. Wright and M.S. El-Shall, Spectroscopy of acetonitrile $(benzene)_n$ clusters, n=1–3. Comparison with benzene clusters 331 (2000) 47
Dantus, M., see Pastirk, I. 333 (2001) 76
Dartois, E., see Pino, T. 339 (2001) 64
Das, P.K., see Kavita, K. 338 (2001) 118
Datskos, P.G., see Lavrik, N.V. 336 (2001) 371
Dávalos, J.Z., see Abboud, J.-L.M. 337 (2001) 327
David Ting, P., see Duda, Y. 339 (2001) 89
Davidson, E.R., see Staroverov, V.N. 340 (2001) 142
Davydov, V.A., L.S. Kashevarova, A.V. Rakhmanina, V.M. Senyavin, O.P. Pronina, N.N. Oleynikov, V. Agafonov, R. Céolin, H. Allouchi and H. Szwarc, Pressure-induced dimerization of fullerene C_{60}: a kinetic study 333 (2001) 224
de Almeida, W.B., see Rocha, W.R. 335 (2001) 127
de Araújo, C.B., see Rakov, N. 332 (2000) 13

Débarre, A., see Azoulay, J. 331 (2000) 347
De Dominicis, L., see Fantoni, R. 332 (2000) 375
de Feraudy, M.-F., see van de Waal, B.W. 331 (2000) 57
de Haas, M.P., see Wegewijs, B.R. 332 (2000) 79
de Jong, P.H.L., see van der Horst, J.-W. 334 (2001) 303
de la Chapelle, M.L., see Tang, C.C. 333 (2001) 12
de Lange, C.A., see Burnell, E.E. 337 (2001) 248
De Luca, F., see Casieri, C. 338 (2001) 137
De Panfilis, C., see Graham, R.G. 332 (2000) 319
de Petris, G. and A. Ricci, Experimental evidence for an asymmetric $Xe_2F_3^+$ ion in the gas-phase 332 (2000) 290
De Schryver, F.C., see Cotlet, M. 336 (2001) 415
De Schryver, F.C., see Hofkens, J. 333 (2001) 255
De Silvestri, S., see Brabec, C.J. 340 (2001) 232
De Silvestri, S., see Cerullo, G. 335 (2001) 27
de Villele, G., see Lewis, E.K. 334 (2001) 357
Deevi, S.C., see Reddy, B.V. 333 (2001) 465
Degli Esposti, A., see Munn, R.W. 336 (2001) 357
Degoricija, L., see Armstrong, J. 332 (2000) 591
Dehez, F., C. Chipot, C. Millot and J.G. Ángyán, Fast and accurate determination of induction energies: reduction of topologically distributed polarizability models 338 (2001) 180
Deka, R.Ch., R. Kinkar Roy and K. Hirao, Basicity of the framework oxygen atom of alkali and alkaline earth-exchanged zeolites: a hard–soft acid–base approach 332 (2000) 576
Delaere, D., M. Tho Nguyen and L.G. Vanquickenborne, A theoretical study on the molecular and electronic structure of heteroaromatic bowl-shaped molecules 333 (2001) 103
Deleuze, M.S., see Claes, L. 339 (2001) 216
Delgado-Barrio, G., see González-Lezana, T. 335 (2001) 105
Demidov, A.A., see Rosca, F. 337 (2001) 107
Demyk, K., see Pino, T. 339 (2001) 64
Deng, F.M., see Chen, X.H. 336 (2001) 201
Deng, J., see Wang, Y. 334 (2001) 411
Dennis, T. John S., see Hino, S. 337 (2001) 65
Dereń, P.J., W. Streęk, E. Zych and J. Drożdżyński, Up-conversion in elpasolite crystals doped with U^{3+} 332 (2000) 308
Derkatch, A., C. Lundevall, L.-E. Berg and P. Royen, Lifetime measurements of the A $^2\Pi$ state of BaCl using laser spectroscopy 332 (2000) 278
Desfrançois, C., see Carles, S. 334 (2001) 374
Devonshire, R., see Payne, D.S. 332 (2000) 58
DeWitt, M.J., see Halls, M.D. 339 (2001) 427
Deyà, P.M., see Quiñonero, D. 339 (2001) 369
Dhathathreyan, A., see Hemakanthi, G. 334 (2001) 245
d'Hendecourt, L., see Pino, T. 339 (2001) 64
di Matteo, A., M. Di Valentin, G. Giacometti and V. Barone, Structure and magnetic properties of aza-aromatic triplet states. The case of quinoxaline 335 (2001) 427
Di Stefano, G. and A. Ricci, Strength of the NF($b^1\Sigma^+ \rightarrow X^3\Sigma^-$) transition. II. Estimate of the NF ground state dissociation limit by analysis of the $\Delta v = 0$ emission sequence 331 (2000) 196
Di Valentin, M., see di Matteo, A. 335 (2001) 427

Dicker, G., see Wegewijs, B.R. 332 (2000) 79
Dickinson, H., T. Chelmick and T.P. Softley, (2+1′) mass analyzed threshold ionization (MATI) spectroscopy of the CD_3 radical 338 (2001) 37
Didenko, O.Z. and P.E. Strizhak, Effect of temperature and small amounts of metal ions on transient chaos in the batch Belousov–Zhabotinsky system 340 (2001) 55
Diep, P., see Kostov, M.K. 332 (2000) 26
Dietz, F., see Tyutyulkov, N. 331 (2000) 465
Dinadayalane, T.C., see Priyakumar, U.D. 336 (2001) 343
Dinadayalane, T.C., see Priyakumar, U.D. 337 (2001) 361
Ding, C.-F., Y. Yu, R.H. Jensen, W.J. Balfour and C.X.W. Qian, Transition metal-chlorine anions and cations: monomers, clusters, and periodic trends 331 (2000) 163
Ding, S. and C.A. McDowell, High resolution ^{23}Na and ^{27}Al NMR satellite transition spectroscopy (SATRAS) of natural sodalite ($Na_8Cl_2(AlSiO_4)_6$) under magic-angle-spinning 333 (2001) 413
Dinse, K.-P., see Goedde, B. 334 (2001) 12
Dirix, G., see Cotlet, M. 336 (2001) 415
Dittrich, T., see Bitzer, T. 331 (2000) 433
Dkhissi, A., R. Ramaekers, L. Houben, L. Adamowicz and G. Maes, DFT/B3-LYP study of the hydrogen-bonding cooperativity: application to $(2\text{-pyridone})_2$, 2-pyridone–H_2O, 2-pyridone–CH_3OH and 2-pyridone–CH_3OCH_3 331 (2000) 553
do Monte, S.A., Effects of Zn and substituents(methyl and *p*-tolyl) on the decay of electron transfer rates in porphyrin–benzene–$(\text{bicyclo[2.2.2]octane})_n$–quinone ($n$=0,1,2) systems 336 (2001) 462
Dobe, C., see Spichiger, D. 337 (2001) 391
Dobrodey, N.V., A.I. Streltsov and L.S. Cederbaum, Interatomic response to core ionization of atomic clusters 339 (2001) 263
Dolg, M., see Hong, G. 334 (2001) 396
Domene, C., P.W. Fowler, M. Wilson, P.A. Madden and R.J. Wheatley, Overlap-model and ab initio cluster calculations of ion properties in distorted environments 333 (2001) 403
Dong, J., see Zhang, L. 335 (2001) 334
Dong, S., see Wu, G. 334 (2001) 265
Dorai, K. and A. Kumar, Fluorine chemical shift tensors in substituted fluorobenzenes using cross correlations in NMR relaxation 335 (2001) 176
Dorozhko, P.A., A.S. Lobach, A.A. Popov, V.M. Senyavin and M.V. Korobov, Sublimation of hydrofullerenes $C_{60}H_{36}$ and $C_{60}H_{18}$ 336 (2001) 39
Douin, S., see Gée, Ch. 338 (2001) 130
Dovesi, R., see Baranek, Ph. 340 (2001) 362
Drake, G.W.F., see Halls, M.D. 339 (2001) 427
Dreesen, L., C. Humbert, P. Hollander, A.A. Mani, K. Ataka, P.A. Thiry and A. Peremans, Study of the water/poly(ethylene glycol) interface by IR-visible sum-frequency generation spectroscopy 333 (2001) 327
Drożdżyński, J., see Dereń, P.J. 332 (2000) 308
Drobizhev, M., A. Karotki and A. Rebane, Persistent spectral hole burning by simultaneous two-photon absorption 334 (2001) 76
Du, C., see Li, Y. 337 (2001) 403
Du, C., see Shi, Z. 336 (2001) 19
Du, J.J., see Wu, X.C. 336 (2001) 53
Du, S., see Li, Y. 335 (2001) 524

Du, Z., see Manos, G. 335 (2001) 77
Duan, W., see Zhou, G. 333 (2001) 344
Dubkov, K.A., see Volodin, A.M. 333 (2001) 41
Dubrovinskaia, N.A., see Dubrovinsky, L.S. 333 (2001) 264
Dubrovinsky, L.S., N.A. Dubrovinskaia, S.K. Saxena, F. Tutti, S. Rekhi, T. Le Bihan, G. Shen and J. Hu, Pressure-induced transformations of cristobalite 333 (2001) 264
Duclaux, L., see Bendiab, N. 339 (2001) 305
Duda, Y., L.L. Lee, Y. Kalyuzhnyi, W.G. Chapman and P. David Ting, Structure and bridge functions of fused-sphere dimeric fluids 339 (2001) 89
Dugourd, P., I. Compagnon, F. Lepine, R. Antoine, D. Rayane and M. Broyer, Beam deviation of large polar molecules in static electric fields: theory and experiment 336 (2001) 511
Duignan, J.P., see Bourhill, G. 336 (2001) 234
Dujardin, C., see Guerassimova, N. 339 (2001) 197
Duncan, M.A., see von Helden, G. 333 (2001) 350
Dunne, L.J., J.N. Murrell and P. Jemmer, Analytical potential energy surface and quasi-classical dynamics for the reaction $LiH(X,^1\Sigma^+)+H(^2S)\rightarrow Li(^2S)+H_2(X,^1\Sigma_g^+)$ 336 (2001) 1
Dunne, L.J., see Manos, G. 335 (2001) 77
Dvorak, J., see Rodriguez, J.A. 336 (2001) 377
Dyke, J.M., see Lee, E.P.F. 340 (2001) 348
Dynarowicz-Łaçtka, P., see Cavalli, A. 338 (2001) 88
Dynarowicz-atka, P., A. Cavalli, D.A. Silva Filho, P. Milart, M. Cristina dos Santos and O.N. Oliveira, Quantitative treatment of surface potentials in Langmuir films from aromatic amphiphiles 337 (2001) 11
Dzuba, S.A., see Borovykh, I.V. 338 (2001) 173

Ebata, T., see Matsumoto, Y. 338 (2001) 52
Ederle, Y., see Koudoumas, E. 335 (2001) 533
Edwards, R., see Stepanek, I. 331 (2000) 125
Egashira, K., Y. Ohshima and O. Kajimoto, Structural characterization of 9-cyanoanthracene–water by rotational coherence spectroscopy 334 (2001) 285
Egorov, V.V., Electron-transfer approach to the nature of the optical lineshape for molecular J-aggregates 336 (2001) 284
Eguchi, T., see Nagasaka, B. 340 (2001) 473
Ehrenberg, B., see Juha, L. 335 (2001) 539
Einaga, H., A. Ogata, S. Futamura and T. Ibusuki, The stabilization of active oxygen species by Pt supported on TiO_2 338 (2001) 303
Eklund, P.C., see Adu, C.K.W. 337 (2001) 31
Eklund, P.C., see Claye, A. 333 (2001) 16
Elguero, J., see Espinosa, E. 336 (2001) 457
Ellis, A.M., see Greetham, G.M. 332 (2000) 303
Elorza, J.M., see Sarasola, C. 337 (2001) 355
El-Shall, M.S., see Daly, G.M. 331 (2000) 47
Emelianova, E.V., see Arkhipov, V.I. 340 (2001) 517
Emura, S., see Iida, S. 338 (2001) 21
Emura, S., see Kubozono, Y. 335 (2001) 163
Endo, Y., see Seki, K. 331 (2000) 184
Engdahl, A., see Nelander, B. 332 (2000) 403
Engdahl, A., see Nelander, B. 339 (2001) 295

Engel, V., see Ermoshin, V.A. 332 (2000) 110
Engel, V., see Ermoshin, V.A. 336 (2001) 262
Engel, V., see Shen, Z. 339 (2001) 362
Engelsberg, M., see Hallwass, F. 335 (2001) 43
Englman, R., see Baer, M. 335 (2001) 85
Engström, M., R. Owenius and O. Vahtras, Ab initio g-tensor calculations of hydrogen bond effects on a nitroxide spin label 338 (2001) 407
Erdmann, M., see Shen, Z. 339 (2001) 362
Ericson, L.M., see Walters, D.A. 338 (2001) 14
Eriksson, O., see Hugosson, H.W. 333 (2001) 444
Ermoshin, V.A. and V. Engel, Manifestation of predissociation and vibrational relaxation in femtosecond pump–probe signals: a theoretical analysis 336 (2001) 262
Ermoshin, V.A. and V. Engel, Stochastic trajectory simulation of femtosecond pump–probe spectroscopy 332 (2000) 110
Espinosa, E., I. Alkorta, I. Rozas, J. Elguero and E. Molins, About the evaluation of the local kinetic, potential and total energy densities in closed-shell interactions 336 (2001) 457
Esposito, F., see Hassouni, K. 340 (2001) 322
Estrada, E., Generalization of topological indices 336 (2001) 248
Estupiñán, E.G., R.E. Stickel and P.H. Wine, An investigation of N_2O production from quenching of $OH(A^2\Sigma^+)$ by N_2 336 (2001) 109
Etchegoin, P., see Burhanudin, Z. 336 (2001) 7
Evans, C.M. and G.L. Findley, Pressure studies of subthreshold photoionization: CH_3I perturbed by CF_4 and c-C_4F_8 337 (2001) 375

Fainberg, B.D., Absorption spectrum of intense chirped pulse by molecules in solution and the time evolution of vibrationally non-equilibrium populations 332 (2000) 181
Faisal, F.H.M., see Muth-Böhm, J. 337 (2001) 313
Falk, K.J., see Shoute, L.C.T. 332 (2000) 359
Fan, J.C., see Lei, Y. 338 (2001) 231
Fan, K., see Wang, Y. 334 (2001) 411
Fan, S.S., see Tang, C.C. 333 (2001) 12
Fan, X.H., L. Xu, C.P. Li, Y.F. Zheng, C.S. Lee and S.T. Lee, Effects of ambient pressure on silicon nanowire growth 334 (2001) 229
Fan, X.H., see Zhang, Z. 337 (2001) 18
Fang, L., X. Shen, X. Chen and J.R. Lombardi, Raman spectra of ruthenium and tantalum trimers in argon matrices 332 (2000) 299
Fang, X., see Peng, X. 340 (2001) 509
Fann, W.S., see White, J.D. 338 (2001) 263
Fantoni, R., M. Giorgi, L. De Dominicis and D.N. Kozlov, Collisional relaxation and internal energy redistribution in NO_2 investigated by means of laser-induced thermal grating technique 332 (2000) 375
Farkas, O., see Torday, L.L. 334 (2001) 381
Farmanara, P., see Stert, V. 337 (2001) 299
Fayer, M.D., see Thompson, D.E. 340 (2001) 267
Fedin, M.V., P A. Purtov and E.G. Bagryanskaya, Anisotropic hyperfine interaction-induced spin relaxation in a low magnetic field 339 (2001) 395
Fedorov, D.G., T. Nakajima and K. Hirao, Analytic gradient for the relativistic elimination of small components (RESCs) approach 335 (2001) 183

Feifel, R., see Hjelte, I. 334 (2001) 151
Feitosa, E., see Cavalli, A. 338 (2001) 88
Feldhaus, J., see Iwanowski, R.J. 336 (2001) 226
Feng, D., see Feng, S. 339 (2001) 103
Feng, M., see Peng, X. 340 (2001) 509
Feng, S., D. Feng, M. Li and Y. Bu, Theoretical studies on the structures and isomerization of methylenelithoflurosilylenoid $H_2C{=}SiLiF$ 339 (2001) 103
Feng, S., see Li, C. 340 (2001) 444
Feng, Z.C., see Guo, Y.P. 339 (2001) 319
Fenn, P.T., see Chen, Y.-J. 336 (2001) 105
Fernández, J.A., see Redondo, C. 331 (2000) 365
Fernández, B., see Bondo Pedersen, T. 334 (2001) 419
Ferri, A., see Polzonetti, G. 340 (2001) 449
Fetisova, Z.G., see Novoderezhkin, V. 335 (2001) 234
Filali-Mouhim, A., see Meesungnoen, J. 335 (2001) 458
Filatov, M. and S. Shaik, Artificial symmetry breaking in radicals is avoided by the use of the Ensemble-Referenced Kohn–Sham (REKS) method 332 (2000) 409
Findley, G.L., see Evans, C.M. 337 (2001) 375
Fink, J., see Jost, O. 339 (2001) 297
Fink, R.F., see Hjelte, I. 334 (2001) 151
Finlayson, C.E., D.S. Ginger and N.C. Greenham, Enhanced Förster energy transfer in organic/inorganic bilayer optical microcavities 338 (2001) 83
Firsov, D.A., B.L. Grigorenko, A.V. Nemukhin, L.Yu. Khriachtchev and M.O. Räsänen, Emission of SH radicals in solid krypton: mixed quantum-classical molecular dynamics simulations 338 (2001) 317
Fischer, B., see Walther, M. 332 (2000) 389
Fischer, J.E., see Claye, A. 333 (2001) 16
Fischer, P., see Champagne, B. 331 (2000) 83
Fitzgerald, G., see Andzelm, J. 335 (2001) 321
Fleming, G.R., see Xu, Q.-H. 338 (2001) 254
Fleming, P.E., E.P.F. Lee and T.G. Wright, The ionization energy and ΔH_f (0 K) of CP, PCP and PCCP 332 (2000) 199
Fleming, P.E., see Armstrong, J. 332 (2000) 591
Fonseca, A., see Pierard, N. 335 (2001) 1
Fowler, J.E., see Sarasola, C. 337 (2001) 355
Fowler, P.W., see Domene, C. 333 (2001) 403
Fowler, P.W., see Rogers, K.M. 332 (2000) 43
Fox, A.M., see Buckley, A.R. 339 (2001) 331
François, J.-P., see Claes, L. 339 (2001) 216
Frankland, S.J.V. and D.W. Brenner, Hydrogen Raman shifts in carbon nanotubes from molecular dynamics simulation 334 (2001) 18
Franklin, N.W., see Zhang, Y. 331 (2000) 35
Frederick, J.H., see Nerukh, D. 332 (2000) 145
Freer, S.T., see Verkhivker, G.M. 336 (2001) 495
Freer, S.T., see Verkhivker, G.M. 337 (2001) 181
Freo, L.D. and A. Painelli, Anharmonicity and NLO responses: artimento an exact diagonalization study 338 (2001) 208
Freyland, W., see Turchanin, A. 337 (2001) 5

Freyland, W., see Zell, C.A. 337 (2001) 293
Friedlein, R., see Jost, O. 339 (2001) 297
Friedlein, R., see Luo, Y. 337 (2001) 176
Frolov, S.V., Ch. Kloc, J.H. Schön and B. Batlogg, Transient spectroscopy of tetracene single crystals 334 (2001) 65
Frontera, A., see Quiñonero, D. 339 (2001) 369
Froudakis, G.E., see Mühlhäuser, M. 336 (2001) 171
Froudakis, G.E., see Schnell, M. 340 (2001) 559
Fu, R., see Ma, Z. 331 (2000) 64
Fuji, T., T. Saito and T. Kobayashi, Dynamical observation of Duschinsky rotation by sub-5-fs real-time spectroscopy 332 (2000) 324
Fujiki, S., see Iida, S. 338 (2001) 21
Fujiwara, A., K. Ishii, H. Suematsu, H. Kataura, Y. Maniwa, S. Suzuki and Y. Achiba, Gas adsorption in the inside and outside of single-walled carbon nanotubes 336 (2001) 205
Fukuhiro, Y., see Kumeda, Y. 333 (2001) 29
Fukunaga, T., see Iida, S. 338 (2001) 21
Fülöp, F., A. Rockenbauer, F. Simon, S. Pekker, L. Korecz, S. Garaj and A. Jánossy, Azafullerene $C_{59}N$, a stable free radical substituent in crystalline C_{60} 334 (2001) 233
Fung, K.K., see Zhang, X.X. 333 (2001) 509
Fung, M.K., Z.Q. Gao, C.S. Lee and S.T. Lee, Inhibition of dark spots growth in organic electroluminescent devices 333 (2001) 432
Furlanetto, M.R., see Pivonka, N.L. 334 (2001) 24
Furube, A., T. Asahi, H. Masuhara, H. Yamashita and M. Anpo, Direct observation of a picosecond charge separation process in photoexcited platinum-loaded TiO_2 particles by femtosecond diffuse reflectance spectroscopy 336 (2001) 424
Furuhashi, O., T. Kinugawa, S. Masuda, C. Yamada and S. Ohtani, Double charge transfer spectroscopy for N_2^{2+} and CO^{2+} at vibrational resolution 337 (2001) 94
Furutani, Y., see Kandori, H. 334 (2001) 271
Futamata, M., Coadsorption of anions and water molecule during underpotential deposition of Cu and Pb on the Au (1 1 1) electrode surface 333 (2001) 337
Futamata, M., Unique adsorbed state of 4,4′-BiPy and -$BiPyH_2^{2+}$ on Au(111) electrode 332 (2000) 421
Futamura, S., see Einaga, H. 338 (2001) 303
Füzéry, A.K., see Torday, L.L. 334 (2001) 381

Gadre, S.R., see Pingale, S.S. 340 (2001) 604
Gaemers, S., see Burnell, E.E. 337 (2001) 248
Gaeta, A.L., see Qiu, J. 333 (2001) 236
Gagliardi, L. and B.O. Roos, Uranium triatomic compounds XUY (X,Y = C,N,O): a combined multiconfigurational second-order perturbation and density functional study 331 (2000) 229
Galander, M., see Savitsky, A.N. 340 (2001) 458
Galaup, J.-P., see Rice, J.H. 335 (2001) 553
Galaup, J.-P., see Schwell, M. 339 (2001) 29
Gálvez, O., P.C. Gómez and L.F. Pacios, Approximate kinetic energy density for intermolecular regions in hydrogen bond dimers 337 (2001) 263
Gan, B., J. Ahn, Q. Zhang, Rusli, S.F. Yoon, J. Yu, Q.-F. Huang, K. Chew, V.A. Ligatchev, X.-B. Zhang and W.-Z. Li, Y-junction carbon nanotubes grown by in situ evaporated copper catalyst 333 (2001) 23

Gan, L., see Zhang, S. 331 (2000) 143
Ganapathi, M.R., S. Naumov, R. Hermann and O. Brede, Nucleophilic effects on the deprotonation of phenol radical cations 337 (2001) 335
Gandy, P.J.F., S. Bardhan, A.L. Mackay and J. Klinowski, Nodal surface approximations to the P,G,D and I-WP triply periodic minimal surfaces 336 (2001) 187
Gangopadhyay, G., see Rana, D. 334 (2001) 314
Gao, E., see Shi, Z. 336 (2001) 19
Gao, K., see Peng, X. 340 (2001) 509
Gao, Y., Y. Chen, X. Ma and C. Chen, Collisional quenching of CCl_2 radicals in the A^1B_1 (0,4,0) and a^3B_1 states by alcohols 339 (2001) 209
Gao, Z.Q., see Fung, M.K. 333 (2001) 432
Garaj, S., see Fülöp, F. 334 (2001) 233
Garashchuk, S., J.C. Light and V.A. Rassolov, The diagonal Born–Oppenheimer correction to molecular dynamical properties 333 (2001) 459
Garau, C., see Quiñonero, D. 339 (2001) 369
García, A.A., see Wegewijs, B.R. 332 (2000) 79
Garcia, E., see Rodriguez, A. 333 (2001) 471
García, G., F. Blanco and A. Williart, Cross-sections for electron scattering by O_2 at intermediate and high energies, 0.1–10 keV 335 (2001) 227
García-Jiménez, F., M.I. Khramov, R. Sánchez-Obregón and O. Collera, Formation of J-aggregates of cyanine dyes in bilayer lipid vesicles 331 (2000) 42
García Solé, J., see Jaque, D. 334 (2001) 309
Garnier, N., see Guerassimova, N. 339 (2001) 197
Garscadden, A., see Haaland, P.D. 340 (2001) 479
Gasmi, K., see Stert, V. 337 (2001) 299
Gavillet, J., see Stepanek, I. 331 (2000) 125
Ge, M., see Wang, J. 340 (2001) 98
Ge, W.K., see Cheng, J. 333 (2001) 375
Gée, Ch., S. Douin, C. Crépin and Ph. Bréchignac, Infrared spectroscopy of aniline ($C_6H_5NH_2$) and its cation in a cryogenic argon matrix 338 (2001) 130
Geen, H., see Heindrichs, A.S.D. 335 (2001) 89
Gehlhaar, D.K., see Verkhivker, G.M. 336 (2001) 495
Gehlhaar, D.K., see Verkhivker, G.M. 337 (2001) 181
Gelinck, G.H., see van der Horst, J.-W. 334 (2001) 303
Geppert, W.D., C. Naulin and M. Costes, Crossed-beam study of the $C(^3P_J)+C_2D_2(X^1\Sigma_g^+) \rightarrow C_3D + D(^2S_{1/2})$ reaction between 4 and 240 meV relative translational energy 333 (2001) 51
Geppert, W.D., see Chastaing, D. 331 (2000) 170
Gerfen, G.J., see Boulet, A.M. 331 (2000) 108
Geum, N. and G.-H. Jeung, Undulating potential curves of the Rydberg states of NaHe 333 (2001) 314
Ghosh, R., see Mandal, S.H. 335 (2001) 281
Giacometti, G., see di Matteo, A. 335 (2001) 427
Gianturco, F.A., see González-Lezana, T. 335 (2001) 105
Gicquel, A., see Hassouni, K. 340 (2001) 322
Giertz, A., see Hjelte, I. 334 (2001) 151
Ginger, D.S., see Finlayson, C.E. 338 (2001) 83

Giordani, C., see Heindrichs, A.S.D. 335 (2001) 89
Giorgi, M., see Fantoni, R. 332 (2000) 375
Glass, G.P., see Sun, F. 337 (2001) 72
Gleeson, M.A., see Lourenço, J.M.C. 336 (2001) 431
Glendening, E.D., see Halpern, A.M. 333 (2001) 391
Glosík, J., R. Plašil, V. Poterya, P. Kudrna and M. Tichý, The recombination of H_3^+ ions with electrons: dependence on partial pressure of H_2 331 (2000) 209
Godt, A., see Jeschke, G. 331 (2000) 243
Goedde, B., M. Waiblinger, P. Jakes, N. Weiden, K.-P. Dinse and A. Weidinger, 'Nitrogen doped' C_{60} dimers ($N@C_{60}$–C_{60}) 334 (2001) 12
Goedert, R.V., T.A. Whittaker, A.F. Clements and G. Bourhill, Imaging the response of an organic nonlinear optical material 332 (2000) 225
Goh, S.H., see Jin, Z. 332 (2000) 461
Goh, S.H., see Jin, Z. 337 (2001) 43
Golden, M.S., see Jost, O. 339 (2001) 297
Goldmann, M., see Haas, H. 335 (2001) 510
Gómez, H., see Liu, Z. 332 (2000) 65
Gómez, P.C., see Gálvez, O. 337 (2001) 263
Gomperts, R., see Abboud, J.-L.M. 337 (2001) 327
Gong, Q., see Li, C. 340 (2001) 444
Gong, X.G. and V. Kumar, Metallic coverings of calcium on C_{60} 334 (2001) 238
González, M., I. Miquel and R. Sayós, VTST kinetics study of the $N(^2D)+O_2(X^3\Sigma_g^-)\rightarrow NO(X^2\Pi)+O(^3P,^1D)$ reactions based on CASSCF and CASPT2 ab initio calculations including excited potential energy surfaces 335 (2001) 339
González-Lezana, T., D. Lopez, S. Miret-Artés, F.A. Gianturco, G. Delgado-Barrio and P. Villarreal, Rotation–vibration interaction in ^{4}He trimers 335 (2001) 105
Gonzalez-Ureña, A., see Stert, V. 337 (2001) 299
Goodson III, T., see Ispasoiu, R.G. 340 (2001) 7
Goossens, A., B. van der Zanden and J. Schoonman, Single-electron migration in nanostructured TiO_2 331 (2000) 1
Gopinath, C.S., see Zaera, F. 332 (2000) 209
Gorbunov, A.A., see Jost, O. 339 (2001) 297
Gordon, A.S., see Yuan, L. 340 (2001) 237
Görling, A., see Sala, F.D. 339 (2001) 343
Gostev, F.E., see Antipin, S.A. 331 (2000) 378
Gough, T.E., T.E. Rowat and T.Y. Wang, An FTIR investigation of co-condensed nitrous oxide, acetylene mixtures. Evidence for two phases with the formula $N_2O \cdot C_2H_2$ 333 (2001) 230
Govindaraj, A., see Murugavel, P. 331 (2000) 149
Govindaraj, A., see Sen, R. 340 (2001) 242
Grabowski, S. J., A new measure of hydrogen bonding strength – ab initio and atoms in molecules studies 338 (2001) 361
Graener, H., see Seifert, G. 333 (2001) 248
Graff, A., see Jost, O. 339 (2001) 297
Grage, M.M.-L., T. Pullerits, A. Ruseckas, M. Theander, O. Inganäs and V. Sundström, Conformational disorder of a substituted polythiophene in solution revealed by excitation transfer 339 (2001) 96

Graham, P., see Tzallas, P. 332 (2000) 236
Graham, R.G., W.M. Holmes, C. De Panfilis and K.J. Packer, Characterisation of locally anisotropic structures within isotropic porous solids using 2-D pulsed field gradient NMR 332 (2000) 319
Grant, E.R., see Clark, J. 340 (2001) 45
Graovac, A., see Gutman, I. 334 (2001) 168
Grätzel, M., see Yoshida, N. 332 (2000) 265
Gray, S.K., B.G. Sumpter, D.W. Noid and M.D. Barnes, Quantum mechanical model of localized electrons on the surface of polymer nanospheres 333 (2001) 308
Greenham, N.C., see Finlayson, C.E. 338 (2001) 83
Greetham, G.M. and A.M. Ellis, The $\tilde{C}$–$\tilde{X}$ electronic spectrum of the SrNC free radical: a jet-cooled investigation 332 (2000) 303
Grigorenko, B.L., see Firsov, D.A. 338 (2001) 317
Grimme, S., Calculation of frequency dependent optical rotation using density functional response theory 339 (2001) 380
Grimme, S., M. Parac and M. Waletzke, On the importance of third- and fourth-order corrections in multi-reference Møller–Plesset theory 334 (2001) 99
Grobert, N., see Mayne, M. 338 (2001) 101
Grobert, N., see Seeger, T. 339 (2001) 41
Gu, B., see Zhou, G. 333 (2001) 344
Gu, J. and J. Leszczynski, The structure, stability, H-bonding pattern, and electrostatic potential of adenine tetrads 335 (2001) 465
Güdel, H.U., see Heer, S. 334 (2001) 293
Guerassimova, N., N. Garnier, C. Dujardin, A.G. Petrosyan and C. Pedrini, X-ray excited charge transfer luminescence of ytterbium-containing aluminium garnets 339 (2001) 197
Guo, H., see Li, G. 336 (2001) 143
Guo, L.C., see He, J.L. 340 (2001) 431
Guo, Q.-X., see Chen, R. 338 (2001) 61
Guo, Q.-X., see Zhang, K.-C. 333 (2001) 195
Guo, Y.P., J.C. Zheng, A.T.S. Wee, C.H.A. Huan, K. Li, J.S. Pan, Z.C. Feng and S.J. Chua, Photoluminescence studies of SiC nanocrystals embedded in a SiO_2 matrix 339 (2001) 319
Guo, Z., see Shi, Z. 336 (2001) 19
Gutman, I., T. Soldatović, A. Graovac and S. Vuković, Approximating the total π-electron energy by means of spectral moments 334 (2001) 168
Gutowski, M., see Skurski, P. 337 (2001) 143
Gutsche, G.J., see Becerra, R. 333 (2001) 83
Guyot-Sionnest, P., see Matranga, C. 340 (2001) 39
Gwóźdź, E., K. Pasterny and A. Bródka, Planar anchoring of polar liquid crystal molecules in slit pore–molecular dynamics simulation study 335 (2001) 71

Ha, T.-K., see Nguyen, M.T. 335 (2001) 311
Haaland, P.D., C.Q. Jiao and A. Garscadden, Ionization of NF_3 by electron impact 340 (2001) 479
Haas, H., W. Caetano, G.P. Borissevitch, M. Tabak, M.I. Mosquera Sanchez, O.N. Oliveira, E. Scalas and M. Goldmann, Interaction of dipyridamole with phospholipid monolayers at the air–water interface: Surface pressure and grazing incidence X-ray diffraction studies 335 (2001) 510

Haas, Y., see Belau, L. 333 (2001) 297
Haber, J., see Brocławik, E. 333 (2001) 332
Hache, F., see Mesnil, H. 338 (2001) 269
Hache, F., see Schanne-Klein, M.C. 338 (2001) 159
Hafner, J., see Benco, L. 333 (2001) 479
Hagen, J., see Socaciu, L.D. 340 (2001) 282
Halabieh, R., see Sultan, R. 332 (2000) 331
Halberstadt, N., see Çarçabal, P. 336 (2001) 335
Halls, M.D., H.B. Schlegel, M.J. DeWitt and G.W.F. Drake, Ab initio calculation of the $a^3\Sigma_u^+$ interaction potential and vibrational levels of $^7Li_2$ 339 (2001) 427
Hallwass, F., M. Engelsberg, A.M. Simas and W. Barros, Diffusion, reaction kinetics and exchange of sodium in aqueous solutions containing a crown ether 335 (2001) 43
Halpern, A.M. and E.D. Glendening, Intrinsic reaction coordinate calculations of the inversion/bending potentials in the $\tilde{X}$ and $\tilde{A}$ states of ammonia 333 (2001) 391
Hamaguchi, H.-o., see Saito, Y. 339 (2001) 351
Hamblett, I., see Monkman, A.P. 340 (2001) 467
Hammes-Schiffer, S., see Iordanov, T. 338 (2001) 389
Hamplová, V., see Juha, L. 335 (2001) 539
Han, J., X. Chen and B.R. Weiner, Reaction dynamics of $O(^3P)+H_2(v=1)$ 332 (2000) 243
Han, K.-L., see Chen, M.-D. 337 (2001) 349
Han, K.-L., see Li, Y.-M. 338 (2001) 297
Han, S., see Lee, C.J. 337 (2001) 398
Hanazaki, I., see Chie, K. 334 (2001) 55
Hancock, G., see Barry, H.R. 333 (2001) 285
Hanf, A., A. Läuter, D. Suresh, H.-R. Volpp and J. Wolfrum, Chlorine atom spin–orbit branching ratios and total absolute reaction cross-sections for the $H + DCl \rightarrow HD + Cl$ reaction 340 (2001) 71
Hankin, S.M., see Tzallas, P. 332 (2000) 236
Hanrath, M. and S.D. Peyerimhoff, The electronic spectrum of C_5 337 (2001) 368
Hansson, T., see Zhang, B. 339 (2001) 438
Hara, Y., see Okazaki, I. 337 (2001) 151
Harigaya, K., New type of antiferromagnetic state in stacked nanographite 340 (2001) 123
Harigaya, K., Tuning of magnetism in stacked nanographite with open shell electrons 339 (2001) 23
Haroz, E.H., see Walters, D.A. 338 (2001) 14
Harper, W.W., S.A. Nizkorodov and D.J. Nesbitt, Differential scattering dynamics of $F+CH_4 \rightarrow HF(v,J)+CH_3$ via high-resolution IR laser dopplerimetry 335 (2001) 381
Hasegawa, J.-y., K. Pierloot and B.O. Roos, Ground state structure of CuO_2: a CASPT2 study 335 (2001) 503
Hashizume, K.-i., see Vacha, M. 331 (2000) 387
Hassouni, K., M. Capitelli, F. Esposito and A. Gicquel, State to state dissociation constants and non-equilibrium vibrational distributions under microwave hydrogen plasmas 340 (2001) 322
Hayashi, H., see Wakasa, M. 340 (2001) 493
Hayazawa, N., Y. Inouye, Z. Sekkat and S. Kawata, Near-field Raman scattering enhanced by a metallized tip 335 (2001) 369
He, G.Z., see Cheng, Y.F. 338 (2001) 308
He, G.-Z., see Li, Y.-M. 338 (2001) 297
He, J.L., see Wang, T.S. 334 (2001) 7

He, J.L., Y.J. Tian, D.L. Yu, T.S. Wang, S.M. Liu, L.C. Guo, D.C. Li, X.P. Jia, L.X. Chen, G.T. Zou and O. Yanagisawa, Orthorhombic B_2CN crystal synthesized by high pressure and temperature 340 (2001) 431
He, S.-G., see Lin, H. 332 (2000) 569
He, T.-J., D.-M. Chen, F.-C. Liu and L.-S. Sheng, The potential energy surface for the decomposition of CH_3OCl 332 (2000) 545
He, Y. and B.J. Orr, Optical heterodyne signal generation and detection in cavity ringdown spectroscopy based on a rapidly swept cavity 335 (2001) 215
He, Z., V. Sundström and T. Pullerits, Excited states of carotenoid in LH2: an ab initio study 334 (2001) 159
Hecht, B., see Segura, J.-M. 340 (2001) 77
Heeger, A.J., see Miller, E.K. 335 (2001) 23
Heer, S., M. Wermuth, K. Krämer and H.U. Güdel, Upconversion excitation of Cr^{3+} ^2E emission in $Y_3Ga_5O_{12}$ codoped with Cr^{3+} and Yb^{3+} 334 (2001) 293
Heid, M., T. Chen, U. Schmitt and W. Kiefer, Spectrally resolved fs-CARS as a probe of the vibrational dynamics of a large polyatomic molecule: magnesium octaethylporphyrin 334 (2001) 119
Heindrichs, A.S.D., H. Geen, C. Giordani and J.J. Titman, Improved scalar shift correlation NMR spectroscopy in solids 335 (2001) 89
Heinonen, M.H., see Iwanowski, R.J. 336 (2001) 226
Heinze, H.H., see Sala, F.D. 339 (2001) 343
Heiz, U., see Socaciu, L.D. 340 (2001) 282
Hellgren, N., see Stafström, S. 340 (2001) 227
Helm, H., see Walther, M. 332 (2000) 389
Hemakanthi, G. and A. Dhathathreyan, Synthesis of nickel sulfide using Langmuir–Blodgett films of nickel complex of 2-hydroxy-5-nitro-*N*-benzylidene hexadecylamine monolayers at air/water interface 334 (2001) 245
Henderson, T.M., K. Runge and R.J. Bartlett, Electron correlation in artificial atoms 337 (2001) 138
Hendrickson, C.L., see Wang, Y. 334 (2001) 69
Hendrickx, M., see Arbuznikov, A.V. 334 (2001) 325
Heninger, M., P. Pernot and H. Mestdagh, Influence of the internal excitation of $FeCO^+$ on its reactivity with O_2 observed in Fourier Transform-ICR cell 333 (2001) 358
Herlin-Boime, N., see Ténégal, F. 335 (2001) 155
Hermann, R., see Ganapathi, M.R. 337 (2001) 335
Hermansson, K., see Baudin, M. 335 (2001) 517
Herrmann, A., see Hofkens, J. 333 (2001) 255
Hess, B., see Walser, R. 334 (2001) 337
Hildebrand, A., see Armstrong, J. 332 (2000) 591
Hill, J., see Buckley, A.R. 339 (2001) 331
Hinde, R.J., M.J. Sepaniak, R.N. Compton, J. Nordling and N. Lavrik, Surface-enhanced resonance Raman scattering of adsorbates under liquid nitrogen 339 (2001) 167
Hino, S., K. Umishita, K. Iwasaki, M. Aoki, K. Kobayashi, S. Nagase, T. John S. Dennis, T. Nakane and H. Shinohara, Ultraviolet photoelectron spectra of metallofullerenes, two $Ca@C_{82}$ isomers 337 (2001) 65
Hirahara, K., see Bandow, S. 337 (2001) 48
Hirano, T., see Kumeda, Y. 333 (2001) 29
Hirao, K., see Deka, R.Ch. 332 (2000) 576
Hirao, K., see Fedorov, D.G. 335 (2001) 183

Hirao, K., see Kobayashi, Y. 336 (2001) 529
Hirao, K., see Qiu, J. 333 (2001) 236
Hirayama, S., see Shoute, L.C.T. 338 (2001) 123
Hirota, N., see Saga, N. 332 (2000) 496
Hitaka, M., see Mito, M. 333 (2001) 69
Hjelte, I., M.N. Piancastelli, R.F. Fink, O. Björneholm, M. Bässler, R. Feifel, A. Giertz, H. Wang, K. Wiesner, A. Ausmees, C. Miron, S.L. Sorensen and S. Svensson, Evidence for ultra-fast dissociation of molecular water from resonant Auger spectroscopy 334 (2001) 151
Hochstrasser, R.M., see Asplund, M.C. 340 (2001) 611
Hockridge, M.R., E.G. Robertson, J.P. Simons, D.R. Borst, T.M. Korter and D.W. Pratt, The $S_1 \leftarrow S_0$ electronic transitions of 4- and 5-phenyl imidazole in the gas phase 334 (2001) 31
Hoff, A.J., see Borovykh, I.V. 338 (2001) 173
Hoffmann, V., see Kurt, R. 335 (2001) 545
Hofkens, J., see Cotlet, M. 336 (2001) 415
Hofkens, J., see Novikov, E. 338 (2001) 151
Hofkens, J., T. Vosch, M. Maus, F. Köhn, M. Cotlet, T. Weil, A. Herrmann, K. Müllen and F.C. De Schryver, Conformational rearrangements in and twisting of a single molecule 333 (2001) 255
Hohage, M., see Lehner, B. 336 (2001) 123
Holas, A., Transforms for idempotency purification of density matrices in linear-scaling electronic-structure calculations 340 (2001) 552
Hollander, P., see Dreesen, L. 333 (2001) 327
Holmes, W.M., see Graham, R.G. 332 (2000) 319
Hong, G., M. Dolg and L. Li, A comparison of scalar-relativistic ZORA and DKH density functional schemes: monohydrides, monooxides and monofluorides of La, Lu, Ac and Lr 334 (2001) 396
Hong, I.P., see Chen, J.M. 337 (2001) 85
Honma, K., see Ideue, S. 337 (2001) 79
Hore, P.J., see Timmel, C.R. 334 (2001) 387
Hori, Y., see Hoshi, N. 336 (2001) 13
Horiai, K., see Ozaki, Y. 335 (2001) 188
Hoshi, N., M. Tanizaki, O. Koga and Y. Hori, Configuration of adsorbed CO affected by the terrace width of Pt(S)-[n(111)×(111)] electrodes 336 (2001) 13
Houben, L., see Dkhissi, A. 331 (2000) 553
Hrbek, J., see Rodriguez, J.A. 336 (2001) 377
Hrušák, J., Some remarks on the stability of the ground and excited electronic states of the CF_2^{++} dication 338 (2001) 189
Hsu, C.-C., see Churikov, V.M. 332 (2000) 19
Hsu, J.H., see White, J.D. 338 (2001) 263
Hu, H., D. Zhang, Y. Liu and C. Liu, Magnetic coupling mechanism in singly bridged binuclear systems 340 (2001) 370
Hu, J., see Dubrovinsky, L.S. 333 (2001) 264
Hu, S.F., see Wang, Y.F. 336 (2001) 47
Hu, T., see Wu, X.C. 336 (2001) 53
Hu, W., see Liu, Y. 331 (2000) 31
Hu, Y., see Li, Y. 333 (2001) 153

Huan, C.H.A., see Guo, Y.P. 339 (2001) 319
Huang, C., see Zhang, S. 331 (2000) 143
Huang, D.-Y., see Xiang, L. 338 (2001) 167
Huang, L., see Jin, Z. 332 (2000) 461
Huang, Q.-F., see Gan, B. 333 (2001) 23
Huang, W., see Li, C. 340 (2001) 444
Huang, Y., see Li, Y. 335 (2001) 524
Huang, Y., see Rutter, M.D. 331 (2000) 189
Huber, J.R., see Li, Q. 334 (2001) 39
Huber, J.R., see Nagai, H. 331 (2000) 425
Hübner, J., see Meskers, S.C.J. 339 (2001) 223
Huczko, A., see Lange, H. 340 (2001) 1
Huffman, C.B., see Walters, D.A. 338 (2001) 14
Hugosson, H.W., U. Jansson, B. Johansson and O. Eriksson, Phase stability diagrams of transition metal carbides, a theoretical study 333 (2001) 444
Huh, Y., see Lee, C.J. 338 (2001) 113
Hultman, L., see Stafström, S. 340 (2001) 227
Humbert, C., see Dreesen, L. 333 (2001) 327
Hummelen, J.C., see Brabec, C.J. 340 (2001) 232
Humphry-Baker, R., see Yoshida, N. 332 (2000) 265
Hung, L.S., see Wong, T.C. 334 (2001) 61
Hung, M.-F., see Churikov, V.M. 332 (2000) 19
Husain, D., see Redondo, C. 331 (2000) 365
Hwang, D.W., see Sinha, A.K. 332 (2000) 455
Hwang, D.-Y. and A.M. Mebel, Reaction mechanism of CO_2 with Ca atom: A theoretical study 331 (2000) 526
Hwang, J.S., see Oweimreen, G.A. 334 (2001) 83
Hwang, L.-P., see Sinha, A.K. 332 (2000) 455

Iarlori, S., see Serra, S. 331 (2000) 339
Ibusuki, T., see Einaga, H. 338 (2001) 303
Ichida, M., see Sakai, M. 335 (2001) 559
Ichihashi, T., see Kokai, F. 332 (2000) 449
Ichikawa, T., see Koizumi, H. 340 (2001) 256
Ichikawa, T., see Takada, T. 335 (2001) 375
Ideue, S., K. Sakamoto, K. Honma and D.E. Clemmer, Conformational change of electrosprayed cytochrome *c* studied by laser-induced fluorescence 337 (2001) 79
Ignatyev, I.S., H.F. Schaefer III and P. von Ragué Schleyer, Triplet states of carbenium and silylium cations 337 (2001) 158
Ignatyev, I.S., H.F. Schaefer III and P. von Ragué Schleyer, Triplet states of carbenium and silylium cations 337 (2001) 169
Ihm, J., see Lee, C.J. 337 (2001) 398
Iida, S., Y. Kubozono, Y. Slovokhotov, Y. Takabayashi, T. Kanbara, T. Fukunaga, S. Fujiki, S. Emura and S. Kashino, Structure and electronic properties of Dy@C_{82} studied by UV–VIS absorption, X-ray powder diffraction and XAFS 338 (2001) 21
Iijima, S., see Azoulay, J. 331 (2000) 347
Iijima, S., see Bandow, S. 337 (2001) 48
Iijima, S., see Kasuya, D. 337 (2001) 25

Iijima, S., see Kokai, F. 332 (2000) 449
Iijima, S., see Murata, K. 331 (2000) 14
Iijima, S., see Sen, R. 340 (2001) 242
Iijima, S., see Zhang, M. 336 (2001) 196
Iimura, K.-i., see Ren, Y. 332 (2000) 339
Iiyama, T., M. Ruike and K. Kaneko, Structural mechanism of water adsorption in hydrophobic micropores from in situ small angle X-ray scattering 331 (2000) 359
Ikushima, Y., see Kanakubo, M. 338 (2001) 95
Ikuyama, R., see Tachibana, M. 332 (2000) 259
Imbihl, R., see Meißen, F. 336 (2001) 181
Improta, R., G. Scalmani and V. Barone, Quantum mechanical prediction of the magnetic titration curve of a nitroxide 'spin probe' 336 (2001) 349
Inaba, A., N. Sakisato and T. Matsuo, Orientationally disordered solid monolayers of tetramethylsilane on graphite and a bilayer nature of the 2-D fluid 340 (2001) 400
Inaba, T., see Zhang, J.-P. 331 (2000) 154
Inaba, T., see Zhang, J.-P. 332 (2000) 351
Inaba, T., see Zhang, J.-P. 340 (2001) 484
Inganäs, O., see Theander, M. 337 (2001) 277
Inganäs, O., see Grage, M.M.-L. 339 (2001) 96
Inouye, Y., see Hayazawa, N. 335 (2001) 369
Ionascu, D., see Rosca, F. 337 (2001) 107
Iordanov, T., S.R. Billeter, S.P. Webb and S. Hammes-Schiffer, Partial multi-dimensional grid generation method for efficient calculation of nuclear wavefunctions 338 (2001) 389
Ishibashi, T.-a., see Yamakata, A. 333 (2001) 271
Ishida, T., see Mito, M. 333 (2001) 69
Ishigaki, T., see Sen, R. 332 (2000) 467
Ishii, K., see Fujiwara, A. 336 (2001) 205
Ishikawa, Y., Y. Sugita, T. Nishikawa and Y. Okamoto, Ab initio replica-exchange Monte Carlo method for cluster studies 333 (2001) 199
Ishikawa, K., see Kimura, T. 340 (2001) 296
Ishikawa, N. and Y. Kaizu, Disappearance of MCD *A* term in the fingerprint band of cation radicals of phthalocyanine metal complexes 339 (2001) 125
Ishikawa, Y. and R.C. Binning Jr., Direct ab initio molecular dynamics study of the protonation of nitric acid 338 (2001) 353
Isobe, H., see Takano, Y. 335 (2001) 395
Ispasoiu, R.G., J. Lee, F. Papadimitrakopoulos and T. Goodson III, Surface effects in the fluorescence ultra-fast dynamics from CdSe nano-crystals 340 (2001) 7
Itaya, A., see Miyasaka, H. 335 (2001) 496
Ito, M., see Nakamura, M. 335 (2001) 170
Ito, M., see Shingaya, Y. 340 (2001) 425
Ito, T., T. Ujiie, M. Naka and H. Nakamura, Photoinduced electron transfer and its magnetic field dependence in supramolecular complex of zinc(II) tetraphenylporphyrin–viologen chain-linked compound with 2,3,6-tri-*O*-methyl-β-cyclodextrin 340 (2001) 308
Itoh, T., A. Matsuyama, K. Maeda and H. Murai, Validity and possibility of photoconductivity-detected magnetic resonance (PCDMR) method as one of reaction-yield-detected magnetic resonance (RYDMR) methods 333 (2001) 242

Iwanowski, R.J., W. Paszkowicz, K. Lawniczak-Jabłońska, M.H. Heinonen, B. Witkowska and J. Feldhaus, Mn–Te bond in the rocksalt $Sn_{1-x}Mn_xTe$ alloys and octahedral radius of Mn: X-Ray absorption- and diffraction study 336 (2001) 226
Iwasaki, K., see Hino, S. 337 (2001) 65

Jain, S.K., C. Rout and R.C. Rastogi, Density functional study of the isomerisation of MOH (M = Be and Mg) 331 (2000) 547
Jakes, P., see Goedde, B. 334 (2001) 12
Jalbout, A.F., Vibrational analysis and ionization potentials of XCH_3 (X = Be, Mg, Ca) calculated by hybrid density functional theory and high order ab initio methods 340 (2001) 571
Jalbout, A.F., see Carles, S. 334 (2001) 374
Jalili, S., see Tafazzoli, M. 331 (2000) 235
Jamieson, D.N., see Prawer, S. 332 (2000) 93
Jánossy, A., see Fülöp, F. 334 (2001) 233
Jansen, M., see Möschel, C. 335 (2001) 9
Jansson, U., see Hugosson, H.W. 333 (2001) 444
Jaque, D. and J. García Solé, Temperature decrease induced by stimulated emission in the Nd^{3+} ion-doped $YAl_3(BO_3)_4$ crystal 334 (2001) 309
Jarzęba, W., S. Pommeret and J.-C. Mialocq, Ultrafast dynamics of the excited methylviologen–iodide charge transfer complexes 333 (2001) 419
Jaschinski, O., see Stepanek, I. 331 (2000) 125
Jaszewski, A.R. and J. Jezierska, An ab initio approach to the structure and EPR parameters of formaldiminoxy radical 334 (2001) 136
Jaszewski, A.R. and J. Jezierska, Hybrid density functional studies on the EPR parameters of heterosubstituted vinyl radicals: substituent effect on the isotropic hyperfine couplings with ^1H and ^{13}C nuclei 340 (2001) 581
Jaszewski, A.R., Z. Siatecki and J. Jezierska, EPR spectroscopy and hybrid density functional studies of dialkoxyphosphinyl-phenyl iminoxy radicals 331 (2000) 403
Jaszuński, M. and K. Ruud, Spin–spin coupling constants in C_2H_2 336 (2001) 473
Jay-Gerin, J.-P., see Meesungnoen, J. 335 (2001) 458
Jeffrey, S.J., see Rasmussen, A.J. 336 (2001) 149
Jemmer, P., see Dunne, L.J. 336 (2001) 1
Jena, P., see Khanna, S.N. 336 (2001) 467
Jensen, R.H., see Ding, C.-F. 331 (2000) 163
Jeong, G.-R., see Li, Z. 340 (2001) 194
Jepsen, P.U., see Walther, M. 332 (2000) 389
Jeschke, G., M. Pannier, A. Godt and H.W. Spiess, Dipolar spectroscopy and spin alignment in electron paramagnetic resonance 331 (2000) 243
Jeung, G.-H., see Geum, N. 333 (2001) 314
Jezierska, J., see Jaszewski, A.R. 331 (2000) 403
Jezierska, J., see Jaszewski, A.R. 334 (2001) 136
Jezierska, J., see Jaszewski, A.R. 340 (2001) 581
Ji, W., see Jin, Z. 332 (2000) 461
Jia, X.P., see He, J.L. 340 (2001) 431
Jia, Z., see Su, H. 335 (2001) 17
Jiang, A.-G., see Xiang, L. 338 (2001) 167
Jiao, C.Q., see Haaland, P.D. 340 (2001) 479

Jin, Z., K.P. Pramada, G. Xu and S.H. Goh, Dynamic mechanical behavior of melt-processed multi-walled carbon nanotube/poly(methyl methacrylate) composites 337 (2001) 43
Jin, Z., L. Huang, S.H. Goh, G. Xu and W. Ji, Characterization and nonlinear optical properties of a poly(acrylic acid)–surfactant–multi-walled carbon nanotube complex 332 (2000) 461
Jirsak, T., see Rodriguez, J.A. 336 (2001) 377
Jochims, H.-W., see Seccombe, D.P. 339 (2001) 405
Johansson, B., see Hugosson, H.W. 333 (2001) 444
Johnson, B.F.G., see Bromley, S.T. 340 (2001) 524
Johnson, J.K., see Kostov, M.K. 332 (2000) 26
Johnson, M.A., see Weber, J.M. 339 (2001) 337
Joo, Y., see Baeck, K.K. 337 (2001) 190
Jost, O., A.A. Gorbunov, J. Möller, W. Pompe, A. Graff, R. Friedlein, X. Liu, M.S. Golden and J. Fink, Impact of catalyst coarsening on the formation of single-wall carbon nanotubes 339 (2001) 297
Joyeux, M., see Sugny, D. 337 (2001) 319
Judai, K., K. Sera, S.-i. Amatsutsumi, K. Yagi, T. Yasuike, S. Yabushita, A. Nakajima and K. Kaya, A soft-landing experiment on organometallic cluster ions: infrared spectroscopy of V(benzene)$_2$ in Ar matrix 334 (2001) 277
Juha, L., B. Ehrenberg, S. Couris, E. Koudoumas, S. Leach, V. Hamplová, Z. Pokorná, A. Müllerová and P. Kubát, Single-photon photolysis of C_{60}, C_{70}, C_{76}, and C_{84} in solutions 335 (2001) 539
Jung, J. and H. Sun, The vibrational structure and predissociation of the B state of $HeBr_2$ using a simple theoretical method 336 (2001) 311

Kadam, R.M., see Bhide, M.K. 332 (2000) 98
Kafafi, Z.H., see Murata, H. 339 (2001) 161
Kafafi, Z.K., see Strohkendl, F.P. 331 (2000) 354
Kais, S., see Sauerwein, R.A. 333 (2001) 451
Kaizu, Y., see Ishikawa, N. 339 (2001) 125
Kajimoto, O., see Egashira, K. 334 (2001) 285
Kallioinen, J., V. Lehtovuori, P. Myllyperkiö and J. Korppi-Tommola, Transient absorption studies of the Ru(dcbpy)$_2$(NCS)$_2$ excited state and the dye cation on nanocrystalline TiO_2 film 340 (2001) 217
Kalyuzhnyi, Y., see Duda, Y. 339 (2001) 89
Kamalakaran, R., see Mayne, M. 338 (2001) 101
Kanada, T., Y. Nishimura, I. Yamazaki and N. Ohta, Electric-field-induced enhancement of LE fluorescence in a linked compound of carbazole and terephthalic acid methyl ester in a PMMA polymer film 332 (2000) 442
Kanakubo, M., T. Umecky, H. Kawanami, T. Aizawa, Y. Ikushima and Y. Masuda, Determination of anisotropic solvation structure of octafluorotoluene in supercritical carbon dioxide by means of solvent-induced ^{19}F NMR chemical shift 338 (2001) 95
Kanbara, T., see Iida, S. 338 (2001) 21
Kandori, H., Y. Furutani, S. Nishimura, Y. Shichida, H. Chosrowjan, Y. Shibata and N. Mataga, Excited-state dynamics of rhodopsin probed by femtosecond fluorescence spectroscopy 334 (2001) 271
Kaneko, K., see Iiyama, T. 331 (2000) 359
Kaneko, K., see Li, D. 335 (2001) 50

Kaneko, K., see Miyawaki, J. 337 (2001) 243
Kaneko, K., see Murata, K. 331 (2000) 14
Kaneko, K., see Tohdoh, A. 340 (2001) 33
Kanno, H., K. Tomikawa and O. Mishima, Reply to the comment on "Raman spectra of low- and high-density amorphous ices" 333 (2001) 324
Karantonis, A., Y. Shiomi and S. Nakabayashi, One-dimensional discrete maps for periodic laser forcing on electrochemical oscillators 335 (2001) 221
Karawajczyk, A., see Rius i Riu, J. 333 (2001) 91
Karawajczyk, A., see Rius i Riu, J. 338 (2001) 285
Karimi, A., see Kurt, R. 335 (2001) 545
Karotki, A., see Drobizhev, M. 334 (2001) 76
Kashevarova, L.S., see Davydov, V.A. 333 (2001) 224
Kashino, S., see Iida, S. 338 (2001) 21
Kashino, S., see Kubozono, Y. 335 (2001) 163
Kasperovich, V., G. Tikhonov and V.V. Kresin, Low-energy electron capture by free C_{60} and the importance of polarization interaction 337 (2001) 55
Kasuya, D., F. Kokai, K. Takahashi, M. Yudasaka and S. Iijima, Formation of C_{60} using CO_2 laser vaporization of graphite at room temperature 337 (2001) 25
Kasuya, D., see Kokai, F. 332 (2000) 449
Kasuya, D., see Sen, R. 332 (2000) 467
Kataura, H., see Fujiwara, A. 336 (2001) 205
Kataura, H., see Sen, R. 332 (2000) 467
Kataura, H., see Sen, R. 340 (2001) 242
Kato, H., see Kudo, A. 331 (2000) 373
Kato, T., see Ren, Y. 332 (2000) 339
Katrusiak, A. and M. Szafrański, Microscopic instabilities related to H_3O^+ dynamics in monoguanidinium dioxonium trinitrate 340 (2001) 302
Kavita, K. and P.K. Das, Dissociation dynamics of fluorinated alkyl iodides at 222 and 236 nm 338 (2001) 118
Kawae, T., see Mito, M. 333 (2001) 69
Kawamata, H., Y. Negishi, A. Nakajima and K. Kaya, Electronic properties of substituted aluminum clusters by boron and carbon atoms ($Al_nB_m^-/Al_nC_m^-$); new insights into *s–p* hybridization and perturbed shell structures 337 (2001) 255
Kawanami, H., see Kanakubo, M. 338 (2001) 95
Kawano, A., see Takahashi, O. 338 (2001) 398
Kawasaki, M., see Sugita, A. 340 (2001) 83
Kawata, M. and M. Mikami, Rapid calculation of two-dimensional Ewald summation 340 (2001) 157
Kawata, M. and U. Nagashima, Particle mesh Ewald method for three-dimensional systems with two-dimensional periodicity 340 (2001) 165
Kawata, M., see Okabe, T. 335 (2001) 435
Kawata, S., see Hayazawa, N. 335 (2001) 369
Kaya, K., see Judai, K. 334 (2001) 277
Kaya, K., see Kawamata, H. 337 (2001) 255
Keheyan, Y., A Fourier-transform ion-cyclotron-resonance study of the reactions of polycyclic aromatic hydrocarbon cations with molecules of interstellar interest 340 (2001) 405
Keiding, S.R., see Poulsen, J. 336 (2001) 488
Keil, M., see Luo, Y. 337 (2001) 176
Keoshian, C.J., see Michael, E.A. 338 (2001) 277

Kerp, H.R. and E.E. van Faassen, Effects of oxygen on exciton transport in zinc phthalocyanine layers 332 (2000) 5
Khan, A., Theoretical studies of $NH_4^+(H_2O)_{20}$ and $NH_3(H_2O)_{20}H^+$ clusters 338 (2001) 201
Khan, K.M. and N. Ahmed, A Monte-Carlo simulation study for the catalytic formation of ammonia 339 (2001) 179
Khanna, S.N. and P. Jena, Magnetic moment and photo-detachment spectroscopy of Ni_5 clusters 336 (2001) 467
Khanna, S.N., see Reddy, B.V. 333 (2001) 465
Khramov, M.I., see García-Jiménez, F. 331 (2000) 42
Khriachtchev, L.Yu., see Firsov, D.A. 338 (2001) 317
Kiefer, W., see Heid, M. 334 (2001) 119
Kim, H.L., see Kim, J.H. 333 (2001) 45
Kim, J., see Weber, J.M. 339 (2001) 337
Kim, J.H. and H.L. Kim, Photodissociation of *s*-triazine at 248 and 193 nm: rotational energy of the HCN fragments 333 (2001) 45
Kim, Y., see Seo, Y. 340 (2001) 186
Kim, Y., see Seo, Y. 340 (2001) 186
Kimmich, R., see Ardelean, I. 332 (2000) 624
Kimura, K., see Yao, H. 340 (2001) 211
Kimura, T., T. Nakamura, K. Ishikawa, F. Kokai and Y. Koga, Time-of-flight mass spectroscopic studies of positive ionic species generated by laser ablation of silicon carbide 340 (2001) 296
Kimura, Y., see Saga, N. 332 (2000) 496
King, K.D., see Becerra, R. 333 (2001) 83
King, R.B., Skyrmion models for three-dimensional aromaticity in deltahedral boranes 338 (2001) 237
King-Smith, R.D., see Andzelm, J. 335 (2001) 321
Kinkar Roy, R., see Deka, R.Ch. 332 (2000) 576
Kinoshita, M., Long-range interaction between hydrophilic surfaces immersed in a hydrophobic fluid containing a hydrophilic component at low concentration 333 (2001) 217
Kinoshita, S., see Watanabe, J. 333 (2001) 113
Kinoshita, S., see Watanabe, Y. 331 (2000) 413
Kinugawa, T., see Furuhashi, O. 337 (2001) 94
Kira, M., see Zeng, H. 331 (2000) 71
Kishimoto, N., see Ohno, K. 332 (2000) 167
Kisiel, Z., B.A. Pietrewicz and L. Pszczółkowski, The experimental electric dipole moments of the Ar_nHX van der Waals clusters 333 (2001) 381
Kitaura, K., S.-I. Sugiki, T. Nakano, Y. Komeiji and M. Uebayasi, Fragment molecular orbital method: analytical energy gradients 336 (2001) 163
Kleiber, P.D., see Lu, W.-Y. 338 (2001) 291
Klenerman, D., see Ying, L. 334 (2001) 145
Kleyn, A.W., see Lourenço, J.M.C. 336 (2001) 431
Klinowski, J., see Gandy, P.J.F. 336 (2001) 187
Kloc, Ch., see Frolov, S.V. 334 (2001) 65
Knapp, E.W., see Saenger, W. 336 (2001) 504
Knijn, A., see Casieri, C. 338 (2001) 137
Knowles, P.J., see Manby, F.R. 335 (2001) 409
Knutson, J.R., see Shen, X. 339 (2001) 191
Kobayashi, K., see Hino, S. 337 (2001) 65

Kobayashi, K., see Kubozono, Y. 335 (2001) 163
Kobayashi, K., see Lu, J. 332 (2000) 219
Kobayashi, T., see Fuji, T. 332 (2000) 324
Kobayashi, Y., H. Nakano and K. Hirao, Multireference Møller–Plesset perturbation theory using spin-dependent orbital energies 336 (2001) 529
Kobayashi, Y., see Tachibana, M. 332 (2000) 259
Koch, H., see Bondo Pedersen, T. 334 (2001) 419
Koch, R., see Schulz, J.J. 331 (2000) 119
Koch, R., see Waldmann, O. 332 (2000) 73
Koehne, J., see Armstrong, J. 332 (2000) 591
Koga, O., see Hoshi, N. 336 (2001) 13
Koga, T., On the extremum property of electron density functions in position and momentum spaces 340 (2001) 547
Koga, Y., see Kimura, T. 340 (2001) 296
Köhn, F., see Hofkens, J. 333 (2001) 255
Köhn, F., see Cotlet, M. 336 (2001) 415
Kohzuma, T., see Nakashima, S. 331 (2000) 396
Koizumi, H., see Takada, T. 335 (2001) 375
Koizumi, H., T. Takada, T. Ichikawa and A. Lund, Photoinduced reactions of 1-(dimethylethyl)-2,2-dimethylpropyl and cyclohexyl radicals in low-temperature solids 340 (2001) 256
Kojima, K., see Tachibana, M. 332 (2000) 259
Kokai, F., K. Takahashi, D. Kasuya, T. Ichihashi, M. Yudasaka and S. Iijima, Synthesis of single-wall carbon nanotubes by millisecond-pulsed CO_2 laser vaporization at room temperature 332 (2000) 449
Kokai, F., see Kasuya, D. 337 (2001) 25
Kokai, F., see Kimura, T. 340 (2001) 296
Kokai, F., see Murata, K. 331 (2000) 14
Komeiji, Y., see Kitaura, K. 336 (2001) 163
Kondo, M., see Kubozono, Y. 335 (2001) 163
Konno, T., see Ozaki, Y. 335 (2001) 188
Konopka, M., see Clark, J. 340 (2001) 45
Konstantaki, M., see Koudoumas, E. 335 (2001) 533
Konya, Z., see Pierard, N. 335 (2001) 1
Koput, J., The equilibrium structure and gas-phase proton affinity of the silanol anion, SiH_3O 333 (2001) 504
Korb, J.-P., A. Van-Quynh and R.G. Bryant, Proton spin relaxation induced by localized spin-dynamical coupling in proteins 339 (2001) 77
Kordatos, K., T.D. Ros, M. Prato, S. Leach, E.J. Land and R.V. Bensasson, Triplet state properties of *N*-mTEG[60]fulleropyrrolidine mono and bisadduct derivatives 334 (2001) 221
Korecz, L., see Fülöp, F. 334 (2001) 233
Kornweitz, H. and A. Persky, Three-center semi-empirical potential energy surfaces for the reactions F+H_2O and F+OH 331 (2000) 132
Korobov, M.V., see Dorozhko, P.A. 336 (2001) 39
Korolkov, M.V. and K.-M. Weitzel, The spin–orbit induced predissociation dynamics of HCl^+ ions: rotational islands of stability 336 (2001) 303
Korppi-Tommola, J., see Kallioinen, J. 340 (2001) 217
Korter, T.M., see Hockridge, M.R. 334 (2001) 31

Kortus, J., M.R. Pederson and S.L. Richardson, First-principles DFT study of the structural, electronic and vibrational properties of azidopentazole 340 (2001) 565
Kosmidis, C., see Tzallas, P. 332 (2000) 236
Kostov, M.K., M.W. Cole, J.C. Lewis, P. Diep and J.K. Johnson, Many-body interactions among adsorbed atoms and molecules within carbon nanotubes and in free space 332 (2000) 26
Kotani, S., see Miyasaka, H. 335 (2001) 496
Koudoumas, E., M. Konstantaki, A. Mavromanolakis, S. Couris, Y. Ederle, C. Mathis, P. Seta and S. Leach, Ultrafast nonlinear optical response of C_{60}–polystyrene star polymers 335 (2001) 533
Koudoumas, E., see Juha, L. 335 (2001) 539
Kovac, J., see Wong, T.C. 334 (2001) 61
Kowalski, A., see Ottinger, Ch. 339 (2001) 53
Kowalski, K. and P. Piecuch, The state-universal multi-reference coupled-cluster theory with perturbative description of core–virtual excitations 334 (2001) 89
Koyama, Y., see Zhang, J.-P. 331 (2000) 154
Koyama, Y., see Zhang, J.-P. 332 (2000) 351
Koyama, Y., see Zhang, J.-P. 340 (2001) 484
Kozlov, D.N., see Fantoni, R. 332 (2000) 375
Kozlowski, P.M., see Andruniow, T. 331 (2000) 502
Kozlowski, P.M., see Andruniow, T. 331 (2000) 509
Kraka, E., see Cremer, D. 337 (2001) 199
Krämer, K., see Heer, S. 334 (2001) 293
Krems, R.V., A.A. Buchachenko, N. Marković and S. Nordholm, On the role of interaction anisotropy in vibrational relaxation of HF and HCl by Ar 335 (2001) 273
Kresin, V.V., see Kasperovich, V. 337 (2001) 55
Kreye, W.C. and P.G. Seybold, Ab initio study of the energetics and thermodynamics of hydrogen abstraction from fluoromethanes by $O(^3P)$. II: $CF_nH_{4-n}+O(^3P)\rightarrow CF_nH_{4-n}\cdots O\rightarrow {}^{\cdot}CF_nH_{3-n}+{}^{\cdot}OH$ (n=0,1,2) 335 (2001) 257
Krishna, R., see Paschek, D. 333 (2001) 278
Krośnicki, M., see Czuchaj, E. 335 (2001) 440
Kroto, H.W., see Mayne, M. 338 (2001) 101
Kroto, H.W., see Seeger, T. 339 (2001) 41
Krylov, A.I., Size-consistent wave functions for bond-breaking: the equation-of-motion spin-flip model 338 (2001) 375
Kubát, P., see Juha, L. 335 (2001) 539
Kubo, S., see Takano, Y. 335 (2001) 395
Kubozono, Y., see Iida, S. 338 (2001) 21
Kubozono, Y., Y. Takabayashi, S. Kashino, M. Kondo, T. Wakahara, T. Akasaka, K. Kobayashi, S. Nagase, S. Emura and K. Yamamoto, Structure of $La_2@C_{80}$ studied by La K-edge XAFS 335 (2001) 163
Kudo, A. and H. Kato, Effect of lanthanide-doping into $NaTaO_3$ photocatalysts for efficient water splitting 331 (2000) 373
Kudrna, P., see Glosík, J. 331 (2000) 209
Kulik, L.V., see Borovykh, I.V. 338 (2001) 173
Kulkarni, G.U., see Raina, G. 337 (2001) 269
Kulkarni, S.A. and R.K. Pathak, Ab initio investigations on neutral clusters of ammonia: $(NH_3)_n$ (n=2–6) 336 (2001) 278

Kumar, A., see Dorai, K. 335 (2001) 176
Kumar, A., see Naik, P.D. 340 (2001) 116
Kumar, A.T.N., see Rosca, F. 337 (2001) 107
Kumar, V., see Gong, X.G. 334 (2001) 238
Kumeda, Y., Y. Fukuhiro, T. Taketsugu and T. Hirano, Theoretical study of nanotube growth in terms of frontier density distribution 333 (2001) 29
Kunkely, H. and A. Vogler, Photoluminescence of flavonolatobis(triphenylphosphine)copper(I) 338 (2001) 29
Kurt, R., A. Karimi and V. Hoffmann, Growth of decorated carbon nano-tubes 335 (2001) 545
Kurushima, N., see Takahashi, O. 338 (2001) 398
Kuwajima, S. and A. Manabe, Computing the rotational viscosity of nematic liquid crystals by an atomistic molecular dynamics simulation 332 (2000) 105
Kuznetsov, V.L., Yu. V. Butenko, A.L. Chuvilin, A.I. Romanenko and A.V. Okotrub, Electrical resistivity of graphitized ultra-disperse diamond and onion-like carbon 336 (2001) 397
Kwon, Y., see Chung, G. 333 (2001) 189

Laarhoven, L.J.J., see Peeters, R. 337 (2001) 231
Laganà, A., see Rodriguez, A. 333 (2001) 471
Lakin, N.M., see Léonard, C. 335 (2001) 97
Lallemand, J.-Y., see Louis-Joseph, A. 337 (2001) 92
Lalowicz, Z.T., see Birczyński, A. 339 (2001) 229
Lan, G.X., see Wang, Y.F. 336 (2001) 47
Land, E.J., see Kordatos, K. 334 (2001) 221
Lang, D.P., see Alam, T.M. 336 (2001) 385
Lange, H. and A. Huczko, Influence of nitrogen on carbon arc plasma and formation of fullerenes 340 (2001) 1
Langenscheidt, A., H. Meyer and A. Schweig, Kinetics of the two-photon ionization of N,N,N′,N′-tetramethylbenzidine in CH_2Cl_2-doped solid argon 331 (2000) 203
Langham, A., see Bentley, J. 332 (2000) 85
Langley, A.J., see Tzallas, P. 332 (2000) 236
Largo, A., see Redondo, P. 335 (2001) 64
Larsen, R.J., see Strohkendl, F.P. 331 (2000) 354
Larson, V., see Verkhivker, G.M. 336 (2001) 495
Larson, V., see Verkhivker, G.M. 337 (2001) 181
Latajka, Z., see Mierzwicki, K. 331 (2000) 538
Latajka, Z., see Panek, J. 332 (2000) 617
Läuter, A., see Hanf, A. 340 (2001) 71
Lavrentovich, O.D., see Smalyukh, I.I. 336 (2001) 88
Lavrik, N., see Hinde, R.J. 339 (2001) 167
Lavrik, N.V., C.A. Tipple, M.J. Sepaniak and P.G. Datskos, Enhanced chemi-mechanical transduction at nanostructured interfaces 336 (2001) 371
Law, C.-K., see Wang, X. 338 (2001) 367
Lawniczak-Jabłońska, K., see Iwanowski, R.J. 336 (2001) 226
Lawrance, W.D., see Becerra, R. 333 (2001) 83
Le Bihan, T., see Dubrovinsky, L.S. 333 (2001) 264
Le Picard, S.D., see Chastaing, D. 331 (2000) 170
Leach, S., see Juha, L. 335 (2001) 539
Leach, S., see Kordatos, K. 334 (2001) 221

Leach, S., see Koudoumas, E. 335 (2001) 533
Leach, S., see Schwell, M. 339 (2001) 29
Lebars, I., see Louis-Joseph, A. 337 (2001) 92
Ledingham, K.W.D., see Tzallas, P. 332 (2000) 236
Leduc, C., see Lewis, E.K. 334 (2001) 357
Lee, C.J., J. Park, S. Han and J. Ihm, Growth and field emission of carbon nanotubes on sodalime glass at 550°C using thermal chemical vapor deposition 337 (2001) 398
Lee, C.J., K.H. Son, J. Park, J.E. Yoo, Y. Huh and J.Y. Lee, Low temperature growth of vertically aligned carbon nanotubes by thermal chemical vapor deposition 338 (2001) 113
Lee, C.J., T.J. Lee and J. Park, Carbon nanofibers grown on sodalime glass at 500°C using thermal chemical vapor deposition 340 (2001) 413
Lee, C.S., see Fan, X.H. 334 (2001) 229
Lee, C.S., see Fung, M.K. 333 (2001) 432
Lee, C.S., see Liao, L.S. 333 (2001) 212
Lee, C.S., see Wong, T.C. 334 (2001) 61
Lee, C.S., see Zhang, Z. 337 (2001) 18
Lee, C.S., see Zhou, X.T. 332 (2000) 215
Lee, E.P.F. and T.G. Wright, A first study of diastatides: $BeAt_2$, BAt_2 and CAt_2 331 (2000) 533
Lee, E.P.F., D.K.W. Mok, J.M. Dyke and F.-T. Chau, Ab initio calculations and spectral simulation of the $\tilde{A}^2A' \rightarrow \tilde{X}^2A''$ emission of the HPCl radical 340 (2001) 348
Lee, E.P.F., J. Lozeille, P. Soldán and T.G. Wright, Calculations on the unstable $CO^-(X^2\Pi)$ anion 336 (2001) 479
Lee, E.P.F., see Fleming, P.E. 332 (2000) 199
Lee, E.P.F., see Wright, T.G. 340 (2001) 179
Lee, J., see Ispasoiu, R.G. 340 (2001) 7
Lee, J.-G., J. Ahner, P. Maksymovych and J.T. Yates Jr, Molecular triangulation – finding the conformation of adsorbed self-assembled organic monolayers 340 (2001) 21
Lee, J.S., Ab initio basis set and correlation limit interaction energies for He–He, He–H_2, and H–H_2 339 (2001) 133
Lee, J.Y., see Lee, C.J. 338 (2001) 113
Lee, L.L., see Duda, Y. 339 (2001) 89
Lee, S.T., see Fan, X.H. 334 (2001) 229
Lee, S.T., see Fung, M.K. 333 (2001) 432
Lee, S.T., see Liao, L.S. 333 (2001) 212
Lee, S.T., see Wong, T.C. 334 (2001) 61
Lee, S.T., see Zhang, Z. 337 (2001) 18
Lee, S.T., see Zhou, X.T. 332 (2000) 215
Lee, T.J., see Lee, C.J. 340 (2001) 413
Lee, Y.-P., see Chen, S.-H. 333 (2001) 365
Lee, Y.-P., see Lo, W.-J. 336 (2001) 71
Lehner, B., M. Hohage and P. Zeppenfeld, Novel Monte Carlo scheme for the simulation of adsorption and desorption processes 336 (2001) 123
Lehtovuori, V., see Kallioinen, J. 340 (2001) 217
Lei, H., H.Z. Wang, Z.C. Wei, X.J. Tang, L.Z. Wu, C.H. Tung and G.Y. Zhou, Photophysical properties and TPA optical limiting of two new organic compounds 333 (2001) 387
Lei, Y., L.D. Zhang and J.C. Fan, Fabrication, characterization and Raman study of TiO_2 nanowire arrays prepared by anodic oxidative hydrolysis of $TiCl_3$ 338 (2001) 231

Leisner, T., see Socaciu, L.D. 340 (2001) 282
Leite, V.B.P., see Bazeia, D. 340 (2001) 205
Lemercier, G., see Mesnil, H. 338 (2001) 269
Lenzer, T., see Pivonka, N.L. 334 (2001) 24
Leo, K., see Agranovich, V.M. 336 (2001) 536
Leon, E., see Boutreau, L. 338 (2001) 74
Léonard, C., D. Panten, N.M. Lakin, G. Chambaud and P. Rosmus, A theoretical study of the Renner–Teller effect in the $\tilde{X}^2\Pi_g$ state of C_3^- 335 (2001) 97
Lepine, F., see Dugourd, P. 336 (2001) 511
Leszczynski, J., see Gu, J. 335 (2001) 465
Leu, G., X.-W. Tang, S. Peled, W.E. Maas, S. Singer, D.G. Cory and P.N. Sen, Amplitude modulation and relaxation due to diffusion in NMR experiments with a rotating sample 332 (2000) 344
Leung, J.W-H., see Shi, Q. 339 (2001) 154
Levesque, D., see Weis, J.-J. 336 (2001) 523
Lewandowski, J., see Pecul, M. 333 (2001) 139
Lewis, E.K., D. Reynolds, X. Li, G. de Villele, C. Leduc, D.L. Cedeño and C. Manzanares I, Phase shift cavity ring-down measurement of C–H ($\Delta v = 6$) vibrational overtone absorptions 334 (2001) 357
Lewis, J.C., see Kostov, M.K. 332 (2000) 26
Leygnier, J., see Bréchignac, C. 335 (2001) 34
Li, C., L. Luo, S. Wang, W. Huang, Q. Gong, Y. Yang and S. Feng, Two-photon microstructure-polymerization initiated by a coumarin derivative/iodonium salt system 340 (2001) 444
Li, C.P., see Fan, X.H. 334 (2001) 229
Li, D. and K. Kaneko, Hydrogen bond-regulated microporous nature of copper complex-assembled microcrystals 335 (2001) 50
Li, D., see Cao, A. 335 (2001) 150
Li, D.C., see He, J.L. 340 (2001) 431
Li, D.C., see Wang, T.S. 334 (2001) 7
Li, F., see Li, Y. 337 (2001) 403
Li, G. and H. Guo, Doubling of Chebyshev correlation function for calculating narrow resonances using low-storage filter diagonalization 336 (2001) 143
Li, G., see Zheng, M. 334 (2001) 298
Li, G.D., see Wang, N. 339 (2001) 47
Li, G.Z. and N. Minami, Photoluminescence from fullerene-doped polyvinylcarbazole (PVK) prepared by solution casting under laser irradiation 331 (2000) 26
Li, J., see Zhou, X. 339 (2001) 117
Li, K., see Guo, Y.P. 339 (2001) 319
Li, K.F., see Meng, J.X. 332 (2000) 313
Li, L., see Hong, G. 334 (2001) 396
Li, L., see Wang, T.S. 334 (2001) 7
Li, M., see Feng, S. 339 (2001) 103
Li, P., see Tang, C.C. 333 (2001) 12
Li, Q., R.T. Carter and J.R. Huber, The photodissociation dynamics of nitric acid studied at 193 nm by LIF and REMPI–TOF methods 334 (2001) 39
Li, Q.-S. and J. Lu, One-dimensional hydrogen atom in quantum phase-space representation: rigorous solutions 336 (2001) 118

Li, R., L.-N.S. Alconcel and R.E. Continetti, Dissociative photodetachment of $SO_2 \cdot SO_2^-$: evidence for the S–O bound dimer 336 (2001) 81
Li, R., W.S. McGivern and S.W. North, Temperature-dependent photodissociation dynamics of ICN at 262 nm 334 (2001) 47
Li, W.-K., see Wang, X. 338 (2001) 367
Li, W.Z., D.Z. Wang, S.X. Yang, J.G. Wen and Z.F. Ren, Controlled growth of carbon nanotubes on graphite foil by chemical vapor deposition 335 (2001) 141
Li, W.Z., see Chen, X.H. 336 (2001) 201
Li, W.-Z., see Gan, B. 333 (2001) 23
Li, X., see Lewis, E.K. 334 (2001) 357
Li, X.-S., see Chen, R. 338 (2001) 61
Li, X.-Y., see Cheng, J. 333 (2001) 375
Li, Y., R. Lu, Y. Hu and X. Wang, Multiphoton ionization and ab initio calculation studies of pyridine–water mixed clusters using time of flight mass spectrometer 333 (2001) 153
Li, Y., S. Wang, F. Li, C. Du, Z. Shi, D. Zhu and Y. Song, Preparation and optical limiting properties of polycarbonates containing fullerene unit 337 (2001) 403
Li, Y., see Borodin, O. 336 (2001) 292
Li, Y., see Chen, H. 335 (2001) 388
Li, Y., see Shi, Z. 336 (2001) 19
Li, Y., see Zhang, X.X. 333 (2001) 509
Li, Y., Y. Huang, S. Du and R. Liu, Structures and stabilities of C_{60}-rings 335 (2001) 524
Li, Y.B., see Sun, L.F. 336 (2001) 392
Li, Y.B., see Sun, L.F. 340 (2001) 222
Li, Y.-M., J.-L. Sun, K.-L. Han and G.-Z. He, Internal-state distribution and polarization in nascent NO $X^2\Pi$ from the photodissociation of C_6H_5NO 338 (2001) 297
Li, Z. and G.-R. Jeong, Ab initio study for reactions of BrO with BrO, OBrO, and Br_2O_2 340 (2001) 194
Li, Z., see Zhang, F. 337 (2001) 125
Li, Z., see Zhang, F. 337 (2001) 131
Li, Z.-H. and M.W. Wong, Scaling of correlation basis set extension energies 337 (2001) 209
Li, Z.Q., see Zhang, X.X. 333 (2001) 509
Li, Z.-s., see Qu, Z.-w. 336 (2001) 325
Li, Z.-s., see Qu, Z.-w. 339 (2001) 140
Liang, C.H., see Wang, Y.W. 339 (2001) 174
Liang, J., see Cao, A. 335 (2001) 150
Liang, K.K., see Villaeys, A.A. 336 (2001) 268
Liao, L.S., X.H. Sun, L.F. Cheng, N.B. Wong, C.S. Lee and S.T. Lee, Ambient effect on the electronic structures of tris-(8-hydroxyquinoline) aluminum films investigated by photoelectron spectroscopy 333 (2001) 212
Liao, X., see Lin, G. 335 (2001) 249
Lichanot, A., see Baranek, Ph. 340 (2001) 362
Lichanot, A., see Tappero, R. 335 (2001) 449
Lidzey, D.G., see Cerullo, G. 335 (2001) 27
Ligatchev, V.A., see Gan, B. 333 (2001) 23
Light, J.C., see Garashchuk, S. 333 (2001) 459
Lim, E.C., see Saigusa, H. 336 (2001) 65
Lim, M., see Asplund, M.C. 340 (2001) 611
Lima, B.H.B., see Bazeia, D. 340 (2001) 205

Lima, C.A.S., M.B.S. Lima, R. Oliva, G. Cardenas and L.C.M. Miranda, Photoacoustic assessment of oscillations in water vapor desorption from nanostructured catalytic surfaces 332 (2000) 428
Lima, M.B.S., see Lima, C.A.S. 332 (2000) 428
Lin, C.-L., M.-D. Su and S.-Y. Chu, Substituent effects on the stabilization of a germanium–sulfur double bond 339 (2001) 147
Lin, D., see Lin, G. 335 (2001) 249
Lin, F., see Zeng, H. 338 (2001) 241
Lin, G., see Chen, Z. 333 (2001) 96
Lin, G., Z. Chen, J. Zhong, D. Lin and X. Liao, A novel propagator approach for NMR signal attenuation due to anisotropic diffusion under various magnetic field gradients 335 (2001) 249
Lin, H., L.-F. Yuan, S.-G. He and X.-G. Wang, Calculating relative intensities for CH stretching polyads of CHI_3 with ab initio dipole moment surface 332 (2000) 569
Lin, J.Y., see Chen, J.M. 337 (2001) 85
Lin, J.Y., see Sun, L.F. 336 (2001) 392
Lin, J.Y., see Sun, L.F. 340 (2001) 222
Lin, M.C., see Moskaleva, L.V. 331 (2000) 269
Lin, P., see McIntosh, A. 331 (2000) 95
Lin, S.H., see Mebel, A.M. 336 (2001) 135
Lin, S.H., see Villaeys, A.A. 336 (2001) 268
Lin, T.-S., see Yang, T.-C. 331 (2000) 489
Linnartz, H., see Bazalgette Courrèges-Lacoste, G. 335 (2001) 209
Lischka, H., see Benco, L. 333 (2001) 479
Liu, C., see Hu, H. 340 (2001) 370
Liu, C., see Zeng, H. 331 (2000) 71
Liu, F.-C., see He, T.-J. 332 (2000) 545
Liu, G., see Cioslowski, J. 331 (2000) 497
Liu, H., see Wang, P. 340 (2001) 261
Liu, L., see Chen, R. 338 (2001) 61
Liu, L., see Zhang, K.-C. 333 (2001) 195
Liu, M., see Peng, X. 340 (2001) 509
Liu, R., see Li, Y. 335 (2001) 524
Liu, S.M., see He, J.L. 340 (2001) 431
Liu, X., see Ahmed, M. 339 (2001) 203
Liu, X., see Jost, O. 339 (2001) 297
Liu, Y., see Hu, H. 340 (2001) 370
Liu, Y., see Walters, K.A. 339 (2001) 255
Liu, Y., see Wang, X. 339 (2001) 36
Liu, Y., see Wang, X. 340 (2001) 419
Liu, Y., see Yu, G. 333 (2001) 207
Liu, Y., W. Hu, X. Wang, C. Long, J. Zhang, D. Zhu, D. Tang and S. Xie, Carbon nanorods 331 (2000) 31
Liu, Y.-G., see Xiang, L. 338 (2001) 167
Liu, Y.Y., see Wang, Y.F. 336 (2001) 47
Liu, Z., H. Gómez and D.M. Neumark, Photoelectron spectroscopy of clustered transition state precursors IHI · Ar and $BrHI^-$ · Ar 332 (2000) 65

Liu, Z.Q., see Sun, L.F. 336 (2001) 392
Liu, Z.Q., see Sun, L.F. 340 (2001) 222
Llanta, E. and R. Rey, Collision-induced absorption in liquid carbon tetrachloride 340 (2001) 173
Lloyd, A.W., see Manby, F.R. 335 (2001) 409
Lluch, J.M., see Torres, L. 340 (2001) 591
Lo, W.-J. and Y.-P. Lee, Ultraviolet absorption spectrum of cyclic CS_2 in solid Ar 336 (2001) 71
Loa, I., see Möschel, C. 335 (2001) 9
Lobach, A.S., see Dorozhko, P.A. 336 (2001) 39
Loh, Z.M., see Wild, D.A. 332 (2000) 531
Loiseau, A., see Stepanek, I. 331 (2000) 125
Lombardi, J.R., see Fang, L. 332 (2000) 299
Long, C., see Liu, Y. 331 (2000) 31
Lopez, D., see González-Lezana, T. 335 (2001) 105
López, M., see Pasqualini, E.E. 336 (2001) 33
López, J.C., see Antolínez, S. 334 (2001) 250
López-Tocón, I., see Pietraperzia, G. 335 (2001) 195
Los, J., see Lourenço, J.M.C. 336 (2001) 431
Lou, N.-Q., see Chen, M.-D. 337 (2001) 349
Louis-Joseph, A., D. Abergel, I. Lebars and J.-Y. Lallemand, Enhancement of water suppression by radiation damping-based manipulation of residual water in Jump and Return NMR experiments 337 (2001) 92
Lourenço, J.M.C., R.T. Carrapa, O.M.N. Teodoro, A.M.C. Moutinho, M.A. Gleeson, J. Los and A.W. Kleyn, Positive and negative ion emission from perfluorinated poly-ethers 336 (2001) 431
Lozeille, J., see Lee, E.P.F. 336 (2001) 479
Lozovik, Yu.E. and A.M. Popov, Erratum to: "Orientational melting of two-shell carbon nanoparticles: molecular dynamics study" [Chemical Physics Letters 328 (2001) 355–362] 335 (2001) 348
Lozovoy, V.V., see Pastirk, I. 333 (2001) 76
Lozovsky, V.A. and S. Cheskis, Intracavity laser absorption spectroscopy study of HNO in hydrocarbon flames doped with N_2O 332 (2000) 508
Lu, J., see Li, Q.-S. 336 (2001) 118
Lu, J., X. Zhang and X. Zhao, Metal-cage hybridization in endohedral $La@C_{60}$, $Y@C_{60}$ and $Sc@C_{60}$ 332 (2000) 51
Lu, J., X. Zhang, X. Zhao, S. Nagase and K. Kobayashi, Strong metal-cage hybridization in endohedral $La@C_{82}$, $Y@C_{82}$ and $Sc@C_{82}$ 332 (2000) 219
Lü, M., see Yang, P. 336 (2001) 76
Lu, R., see Li, Y. 333 (2001) 153
Lu, W.-Y. and P.D. Kleiber, Photochemical dynamics of Mg^+-acetaldehyde: C–H vs. C–C bond activation pathways 338 (2001) 291
Lu, Y., see Xie, D. 339 (2001) 14
Lucchese, R.R., see McIntosh, A. 331 (2000) 95
Luh, T.-Y., see Churikov, V.M. 332 (2000) 19
Luna, A., see Boutreau, L. 338 (2001) 74
Lund, A., see Koizumi, H. 340 (2001) 256
Lund, A., see Takada, T. 335 (2001) 375

Lund, A., see Volodin, A.M. 333 (2001) 41
Lundell, J., G.M. Chaban and R. Benny Gerber, Combined ab initio and anharmonic vibrational spectroscopy calculations for rare gas containing fluorohydrides, HRgF 331 (2000) 308
Lundevall, C., see Derkatch, A. 332 (2000) 278
Luo, L., see Li, C. 340 (2001) 444
Luo, Y., H. Ågren, M. Keil, R. Friedlein and W.R. Salaneck, A theoretical investigation of the near-edge X-ray absorption spectrum of hexa-*peri*-hexabenzocoronene 337 (2001) 176
Luque, F.J., see Chipot, C. 332 (2000) 190
Luty, B.A., see Verkhivker, G.M. 336 (2001) 495
Luty, B.A., see Verkhivker, G.M. 337 (2001) 181
Luzzati, S., see Brabec, C.J. 340 (2001) 232
Luzzi, D.E., see Smith, B.W. 331 (2000) 137

Ma, F., see Sun, M. 339 (2001) 413
Ma, R., Y. Bando and T. Sato, CVD synthesis of boron nitride nanotubes without metal catalysts 337 (2001) 61
Ma, S., see Resmi, M.R. 333 (2001) 515
Ma, S.Y., Theoretical studies on the structural change in the *N*-protonated *meso*-tetrakis(*p*-sulfonatophenyl)porphyrin 332 (2000) 603
Ma, X., see Gao, Y. 339 (2001) 209
Ma, X., see Zhou, X. 339 (2001) 117
Ma, X.C., see Sun, L.F. 336 (2001) 392
Ma, X.C., see Sun, L.F. 340 (2001) 222
Ma, Y.-Z., see Xu, Q.-H. 338 (2001) 254
Ma, Z., J.P. Zheng and R. Fu, Solid state NMR investigation of hydrous ruthenium oxide 331 (2000) 64
Maas, W.E., see Leu, G. 332 (2000) 344
Machado, J.C., see Marques-Netto, A. 333 (2001) 371
Mackay, A.L., see Gandy, P.J.F. 336 (2001) 187
Mackenzie, S.R., see Monti, O.L.A. 333 (2001) 146
Madden, P.A., see Domene, C. 333 (2001) 403
Maeda, K., see Araki, Y. 332 (2000) 515
Maeda, K., see Itoh, T. 333 (2001) 242
Maes, G., see Dkhissi, A. 331 (2000) 553
Magnier, S. and A. Toniolo, Above threshold dissociation of $LiNa^+$: monitoring an avoided crossing with femtosecond spectroscopy 338 (2001) 329
Maiti, A., Mechanical deformation in carbon nanotubes – bent tubes vs tubes pushed by atomically sharp tips 331 (2000) 21
Maiti, A., see Rodriguez, J.A. 336 (2001) 377
Maksymovych, P., see Lee, J.-G. 340 (2001) 21
Malliaras, G.G., see Murata, H. 339 (2001) 161
Mallick, P.K., see Sett, P. 331 (2000) 215
Malta, O.L., see Albuquerque, R.Q. 331 (2000) 519
Manaa, M.R., Toward new energy-rich molecular systems: from N_{10} to N_{60} 331 (2000) 262
Manabe, A., see Kuwajima, S. 332 (2000) 105
Mančal, T. and V. May, Non-Markovian dissipation of molecular vibrational energy via multi-quantum processes 334 (2001) 179

Manas, E.S. and L.X. Chen, Electronic interactions in metal complexed photoconducting polymers: a ZINDO study 331 (2000) 299
Manby, F.R., P.J. Knowles and A.W. Lloyd, Density matrix functional theory in average and relative coordinates 335 (2001) 409
Mandal, S.H., R. Ghosh and D. Mukherjee, A non-perturbative cumulant expansion method for the grand partition function of quantum systems 335 (2001) 281
Mango, F., see Bernheim, R.A. 332 (2000) 1
Mani, A.A., see Dreesen, L. 333 (2001) 327
Maniwa, Y., see Fujiwara, A. 336 (2001) 205
Mankhetkorn, S., see Meesungnoen, J. 335 (2001) 458
Manos, G., L.J. Dunne, M.F. Chaplin and Z. Du, Comparative study of Monte Carlo simulations and exact statistical mechanical lattice model of commensurate transitions of alkanes adsorbed in zeolites 335 (2001) 77
Manzanares I, C., see Lewis, E.K. 334 (2001) 357
Mao, S., see Zeng, H. 338 (2001) 241
Marevtsev, V.S., see Antipin, S.A. 331 (2000) 378
Mark, A.E., see Walser, R. 334 (2001) 337
Marković, N., see Krems, R.V. 335 (2001) 273
Maroulis, G., Accurate higher electric multipole moments for carbon monoxide 334 (2001) 214
Maroulis, G., On the static electric polarizability and hyperpolarizability of sodium. How good is the agreement between theory and experiment for the dipole polarizability? 334 (2001) 207
Marques-Netto, A., C.F. Carvalho, C.A. Alves de Carvalho, R.D. Sinisterra, H.F. Brito and J.C. Machado, Positronium formation in lanthanide (III) trifluoroacetate with 3-picoline-N-oxide compounds 333 (2001) 371
Marrone, T., see Verkhivker, G.M. 336 (2001) 495
Marrone, T., see Verkhivker, G.M. 337 (2001) 181
Marsh, R.J. and A.J. McCaffery, Rotational transfer in diatom–diatom collisions 335 (2001) 134
Marshall, A.G., see Wang, Y. 334 (2001) 69
Martínez-Núñez, E. and S.A. Vázquez, Three-center vs. four-center HF elimination from vinyl fluoride: a direct dynamics study 332 (2000) 583
Martí, V., see Adam, W. 340 (2001) 26
Martin, J.-P., M.-Y. Perrin and P.I. Porshnev, CO_2 formation in an optically excited V–V up-pumped CO flow 332 (2000) 283
Martin, M.M., see Changenet-Barret, P. 336 (2001) 439
Martin, R.L., see Tretiak, S. 331 (2000) 561
Martinho, J.M.G., see Bodunov, E.N. 340 (2001) 137
Martins, J.B.L., see Beltrán, A. 338 (2001) 224
Masamura, M., Ab initio molecular orbital study of $OH^-(H_2O)_n$ and $SH^-(H_2O)_n$ in the gas phase 339 (2001) 279
Maschmeyer, Th., see Bromley, S.T. 340 (2001) 524
Masella, M., see Vitorge, P. 332 (2000) 367
Massobrio, C., see Pouillon, Y. 331 (2000) 290
Masuda, S., see Furuhashi, O. 337 (2001) 94
Masuda, Y., see Kanakubo, M. 338 (2001) 95
Masuhara, H., see Furube, A. 336 (2001) 424
Mataga, N., see Kandori, H. 334 (2001) 271
Mathis, C., see Koudoumas, E. 335 (2001) 533

Matranga, C. and P. Guyot-Sionnest, Intermolecular vibrational energy transfer between cyanide species at the platinum/electrolyte interface 340 (2001) 39
Matsui, H., see Shiina, H. 336 (2001) 242
Matsumi, Y., see Sugita, A. 340 (2001) 83
Matsumoto, Y., T. Ebata and N. Mikami, OH stretching vibrations and hydrogen-bonded structures of 7-hydroxyquinoline-$(H_2O)_{1-3}$ investigated by IR–UV double-resonance spectroscopy 338 (2001) 52
Matsuo, T., see Inaba, A. 340 (2001) 400
Matsuyama, A., see Itoh, T. 333 (2001) 242
Maurin, G., see Stepanek, I. 331 (2000) 125
Maus, M., see Hofkens, J. 333 (2001) 255
Mavridis, A., see Metropoulos, A. 331 (2000) 89
Mavridis, A., see Tzeli, D. 340 (2001) 538
Mavromanolakis, A., see Koudoumas, E. 335 (2001) 533
May, V., see Mančal, T. 334 (2001) 179
Mayanovic, R.A., A.J. Anderson, W.A. Bassett and I.-M. Chou, Hydrogen bond breaking in aqueous solutions near the critical point 336 (2001) 212
Mayer, I., A chemical energy component analysis 332 (2000) 381
Mayer, I., see Sauge, S. 334 (2001) 330
Mayne, M., N. Grobert, M. Terrones, R. Kamalakaran, M. Rühle, H.W. Kroto and D.R.M. Walton, Pyrolytic production of aligned carbon nanotubes from homogeneously dispersed benzene-based aerosols 338 (2001) 101
Mayne, M., see Ténégal, F. 335 (2001) 155
Mazziotti, D.A., Energy functional of the one-particle reduced density matrix: a geminal approach 338 (2001) 323
McCaffery, A.J., see Marsh, R.J. 335 (2001) 134
McCanny, T., see Tzallas, P. 332 (2000) 236
McDouall, J.J.W., see Bramwell, M.J. 331 (2000) 483
McDowell, C.A., see Ding, S. 333 (2001) 413
McGivern, W.S., see Li, R. 334 (2001) 47
McIntosh, A., P. Lin, R.R. Lucchese, J.W. Bevan, D.J. Brugh and R.D. Suenram, The microwave spectrum and ground state dynamics of Kr–IH 331 (2000) 95
Mebel, A.M., M. Baer, V.M. Rozenbaum and S.H. Lin, Ab initio study of nonadiabatic coupling matrix elements between excited $2^2A'$ and $3^2A'$ electronic states of C_2H 336 (2001) 135
Mebel, A.M., see Hwang, D.-Y. 331 (2000) 526
Meesungnoen, J., J.-P. Jay-Gerin, A. Filali-Mouhim and S. Mankhetkorn, Monte-Carlo calculation of the primary $H^{\cdot}$ atom yield in liquid water radiolysis: effects of radiation type and temperature 335 (2001) 458
Meißen, F., A.J. Patchett, R. Imbihl and A.M. Bradshaw, Novel types of spatio-temporal patterns in catalytic CO oxidation on a facetted Pt(110) surface 336 (2001) 181
Meier, R., see Spichiger, D. 337 (2001) 391
Meijer, E.J., see van Erp, T.S. 333 (2001) 290
Meijer, G., see Peeters, R. 337 (2001) 231
Meijer, G., see von Helden, G. 333 (2001) 350
Melikyan, A. and H. Minassian, Phonon confinement in ultrathin nickel films 331 (2000) 115
Mellouki, A., see Yujing, M. 333 (2001) 63
Meng, G.W., see Wang, Y.W. 339 (2001) 174

Meng, J.X., K.F. Li, J. Yuan, L.L. Zhang, W.K. Wong and K.W. Cheah, Near-IR luminescence and photophysics of Yb-porphyrinate complexes 332 (2000) 313
Mérawa, M., D. Bégué, M. Rérat and C. Pouchan, Long-range dispersion coefficients for the low-lying electronic states of Mg_2 from the calculation of the frequency-dependent dipole polarizabilities of Mg in its ground and excited states 334 (2001) 403
Merchant, K.A., see Thompson, D.E. 340 (2001) 267
Meskers, S.C.J., J. Hübner, M. Oestreich and H. Bässler, Time-resolved fluorescence studies and Monte Carlo simulations of relaxation dynamics of photoexcitations in a polyfluorene film 339 (2001) 223
Mesnil, H., M.C. Schanne-Klein, F. Hache, M. Alexandre, G. Lemercier and C. Andraud, Experimental observation of nonlinear circular dichroism in a pump–probe experiment 338 (2001) 269
Mestdagh, H., see Heninger, M. 333 (2001) 358
Metropoulos, A. and A. Mavridis, Predissociation lifetimes of the $E^2\Pi$ and $F^2\Pi$ states of CH 331 (2000) 89
Meyer, H., see Langenscheidt, A. 331 (2000) 203
Meyer, K.A., see Murdoch, K.M. 335 (2001) 349
Mialocq, J.-C., see Jarzęba, W. 333 (2001) 419
Miani, A., see Cané, E. 340 (2001) 356
Michael, E.A., C.J. Keoshian, D.R. Wagner, S.K. Anderson and R.J. Saykally, Infrared water recombination lasers 338 (2001) 277
Michels, M.A.J., see van der Horst, J.-W. 334 (2001) 303
Michiels, J., see Cotlet, M. 336 (2001) 415
Mierzwicki, K., S. Berski and Z. Latajka, Nature of chemical bonds in MCCH (M = Li, Na, K) based on the topological analysis of electron localisation function (ELF) and electron density 331 (2000) 538
Mikami, M., see Kawata, M. 340 (2001) 157
Mikami, M., see Okabe, T. 335 (2001) 435
Mikami, M., see Shinoda, W. 335 (2001) 265
Mikami, N., see Matsumoto, Y. 338 (2001) 52
Milart, P., see Dynarowicz-atka, P. 337 (2001) 11
Milas, I. and M.A.C. Nascimento, A density-functional study of the dehydrogenation reaction of isobutane over zeolites 338 (2001) 67
Millefiori, S. and A. Alparone, Second hyperpolarisability of furan homologues C_4H_4X (X = O, S, Se, Te): ab initio HF and DFT study 332 (2000) 175
Miller, E.K., C.J. Brabec, H. Neugebauer, A.J. Heeger and N. Serdar Sariciftci, Polarized doping-induced infrared absorption in highly oriented conjugated polymers 335 (2001) 23
Miller, J., see Rakov, N. 332 (2000) 13
Miller, M.A., L.M. Amon and W.P. Reinhardt, Should one adjust the maximum step size in a Metropolis Monte Carlo simulation? 331 (2000) 278
Miller, T.A., see Zalyubovsky, S.J. 335 (2001) 298
Millié, P., see Çarçabal, P. 336 (2001) 335
Millot, C., see Dehez, F. 338 (2001) 180
Milman, V., see Winkler, B. 337 (2001) 36
Minami, N., see Li, G.Z. 331 (2000) 26
Minassian, H., see Melikyan, A. 331 (2000) 115
Miquel, I., see González, M. 335 (2001) 339

Miranda, L.C.M., see Lima, C.A.S. 332 (2000) 428
Miret-Artés, S., see González-Lezana, T. 335 (2001) 105
Miron, C., see Hjelte, I. 334 (2001) 151
Mishima, O., see Kanno, H. 333 (2001) 324
Mito, M., T. Kawae, M. Hitaka, K. Takeda, T. Ishida and T. Nogami, Pressure effects of genuine organic crystalline ferromagnet possessing intermolecular contacts between nitroxide oxygen and methyl hydrogen atoms 333 (2001) 69
Mitsutake, A. and Y. Okamoto, Replica-exchange simulated tempering method for simulations of frustrated systems 332 (2000) 131
Mittal, J., M. Monthioux, H. Allouche and O. Stephan, Room temperature filling of single-wall carbon nanotubes with chromium oxide in open air 339 (2001) 311
Mittal, J.P., see Naik, P.D. 340 (2001) 116
Miura, A., see Yang, X. 334 (2001) 257
Miura, S., see Shiga, M. 332 (2000) 396
Miura, S., see Shinoda, K. 337 (2001) 306
Miyasaka, H., S. Kotani, T. Ota and A. Itaya, Formation of extremely long-lived charge-separated state by two-photon ionization in poly(*N*-vinylcarbazole) adsorbed on a macroreticular resin 335 (2001) 496
Miyawaki, J. and K. Kaneko, Pore width dependence of the temperature change of the confined methane density in slit-shaped micropores 337 (2001) 243
Miyoshi, A., see Shiina, H. 336 (2001) 242
Möbius, K., see Savitsky, A.N. 340 (2001) 458
Mochizuki, Y. and H. Ågren, Polarizability of silicon clusters 336 (2001) 451
Mohallem, J.R., see Rolim, F. 332 (2000) 139
Mok, D.K.W., see Lee, E.P.F. 340 (2001) 348
Molins, E., see Espinosa, E. 336 (2001) 457
Möller, J., see Jost, O. 339 (2001) 297
Monkman, A.P., H.D. Burrows, I. Hamblett and S. Navaratnam, Intra-chain triplet–triplet annihilation and delayed fluorescence in soluble conjugated polymers 340 (2001) 467
Monthioux, M., see Mittal, J. 339 (2001) 311
Monti, O.L.A., H.A. Cruse, T.P. Softley and S.R. Mackenzie, High resolution photoionisation spectroscopy of vibrationally excited Ar·NO 333 (2001) 146
Moraes, F., see Bazeia, D. 340 (2001) 205
Moraldi, M., see Ceccherini, S. 337 (2001) 386
Moreno, M., see Torres, L. 340 (2001) 591
Moroi, Y., see Yoshida, N. 332 (2000) 265
Möschel, C., A. Reich, W. Assenmacher, I. Loa and M. Jansen, Onion-like marbles and bats: new morphological forms of carbon 335 (2001) 9
Moskaleva, L.V., W.S. Xia and M.C. Lin, The CH+N_2 reaction over the ground electronic doublet potential energy surface: a detailed transition state search 331 (2000) 269
Mosquera Castro, R.A., see Cioslowski, J. 331 (2000) 497
Mosquera Sanchez, M.I., see Haas, H. 335 (2001) 510
Mosquera, R.A., see Vila, A. 332 (2000) 474
Mostafavi, M., see Renou, F. 335 (2001) 363
Moszynski, R., see Rode, M. 334 (2001) 424
Motylewski, T., see Bazalgette Courrèges-Lacoste, G. 335 (2001) 209
Moutinho, A.M.C., see Lourenço, J.M.C. 336 (2001) 431
Mu, T.-W., see Zhang, K.-C. 333 (2001) 195

Muhammed, M., see Baudin, M. 335 (2001) 517
Mühlhäuser, M., see Schnell, M. 340 (2001) 559
Mühlhäuser, M., G.E. Froudakis and S.D. Peyerimhoff, MRD-CI study of the electronic spectrum of linear C_9 336 (2001) 171
Mukai, K. and S. Abe, Effects of positional disorder on optical absorption spectra of light-harvesting antenna complexes in photosynthetic bacteria 336 (2001) 445
Mukherjee, D., see Mandal, S.H. 335 (2001) 281
Müllen, K., see Hofkens, J. 333 (2001) 255
Müllen, K., see Tyutyulkov, N. 331 (2000) 465
Müller, P., see Waldmann, O. 332 (2000) 73
Müllerová, A., see Juha, L. 335 (2001) 539
Muniz-Miranda, M., On the occurrence of the central line (~1025 cm^{-1}) in the SERS spectra of pyridine adsorbed on silver hydrosols 340 (2001) 437
Munn, R.W., M. Andrzejak, P. Petelenz, A. Degli Esposti and C. Taliani, Calculation of refractive indices and local electric field tensors in α-sexithiophene crystal 336 (2001) 357
Murai, H., see Araki, Y. 332 (2000) 515
Murai, H., see Itoh, T. 333 (2001) 242
Murakami, J., see Tai, Y. 339 (2001) 9
Murata, H., G.G. Malliaras, M. Uchida, Y. Shen and Z.H. Kafafi, Non-dispersive and air-stable electron transport in an amorphous organic semiconductor 339 (2001) 161
Murata, K., K. Kaneko, F. Kokai, K. Takahashi, M. Yudasaka and S. Iijima, Pore structure of single-wall carbon nanohorn aggregates 331 (2000) 14
Murdoch, K.M., N.J. Condon, W. Zhao, D.M. Besemann, K.A. Meyer and J.C. Wright, Isotope and mode selectivity in two-dimensional vibrational four wave mixing spectroscopy 335 (2001) 349
Murrell, J.N., see Dunne, L.J. 336 (2001) 1
Murugavel, P., C. Narayana, A. Govindaraj, A.K. Sood and C.N.R. Rao, Brillouin scattering from C_{70} and C_{60} films: a comparative study of elastic properties 331 (2000) 149
Muth-Böhm, J., A. Becker, S.L. Chin and F.H.M. Faisal, *S*-matrix theory of ionisation of polyatomic molecules in an intense laser pulse 337 (2001) 313
Mutzenhardt, P., see Ancian, B. 336 (2001) 410
Myllyperkiö, P., see Kallioinen, J. 340 (2001) 217

Nachimuthu, P., see Chen, J.M. 337 (2001) 85
Nagai, H., R.T. Carter and J.R. Huber, Spectroscopy and dynamics of selected rotational levels in the $\tilde{B}^2A''$ state of the vinoxy radical 331 (2000) 425
Nagaoka, M., see Okazaki, I. 337 (2001) 151
Nagaoka, M., see Yamaguchi, Y. 340 (2001) 129
Nagasaka, B., H. Omi, T. Eguchi, H. Nakayama and N. Nakamura, High-pressure ^{129}XeNMR study of supercritical xenon interacting with polymers 340 (2001) 473
Nagasawa, Y., see Nakashima, S. 331 (2000) 396
Nagase, S., see Hino, S. 337 (2001) 65
Nagase, S., see Kubozono, Y. 335 (2001) 163
Nagase, S., see Lu, J. 332 (2000) 219
Nagashima, U., see Kawata, M. 340 (2001) 165
Nagata, T., see Saeki, M. 340 (2001) 376
Nagy, Á. and K.D. Sen, Exact results on the curvature of the electron density at the cusp in certain highly excited states of atoms 332 (2000) 154

Nagy, J.B., see Pierard, N. 335 (2001) 1
Naik, P.D., H.P. Upadhyaya, A. Kumar, A.V. Sapre and J.P. Mittal, Dynamics of acetic acid dissociation at 193.3 nm: selectivity in OH reaction channel 340 (2001) 116
Naito, S., see Shimizu, O. 332 (2000) 295
Naka, M., see Ito, T. 340 (2001) 308
Nakabayashi, S., see Karantonis, A. 335 (2001) 221
Nakajima, A., see Judai, K. 334 (2001) 277
Nakajima, A., see Kawamata, H. 337 (2001) 255
Nakajima, T., see Fedorov, D.G. 335 (2001) 183
Nakamura, A., see Sakai, M. 335 (2001) 559
Nakamura, H., see Ito, T. 340 (2001) 308
Nakamura, M. and M. Ito, Coadsorption of water monomers with CO on Ru(001) and charge transfer during hydration processes 335 (2001) 170
Nakamura, N., see Nagasaka, B. 340 (2001) 473
Nakamura, T., see Kimura, T. 340 (2001) 296
Nakane, T., see Hino, S. 337 (2001) 65
Nakano, H., see Kobayashi, Y. 336 (2001) 529
Nakano, T., see Kitaura, K. 336 (2001) 163
Nakashima, S., Y. Nagasawa, K. Seike, T. Okada, M. Sato and T. Kohzuma, Coherent dynamics in ultrafast charge-transfer reaction of plastocyanin 331 (2000) 396
Nakayama, H., see Nagasaka, B. 340 (2001) 473
Narahari Sastry, G., see Priyakumar, U.D. 336 (2001) 343
Narayana, C., see Murugavel, P. 331 (2000) 149
Narayana, C., see Sudheendra, L. 340 (2001) 275
Nascimento, M.A.C., see Milas, I. 338 (2001) 67
Natarajan, V., see Bhide, M.K. 332 (2000) 98
Nattland, D., see Turchanin, A. 337 (2001) 5
Naulin, C., see Chastaing, D. 331 (2000) 170
Naulin, C., see Geppert, W.D. 333 (2001) 51
Naumov, S., see Ganapathi, M.R. 337 (2001) 335
Navaratnam, S., see Monkman, A.P. 340 (2001) 467
Negishi, Y., see Kawamata, H. 337 (2001) 255
Nelander, B., A. Engdahl and T. Svensson, The HOOO radical. A matrix isolation study 332 (2000) 403
Nelander, B., A. Engdahl and T. Svensson, The HOOO radical. A matrix isolation study [Chem. Phys. Lett. 332 (2000) 403] 339 (2001) 295
Nemukhin, A.V., see Firsov, D.A. 338 (2001) 317
Nerukh, D. and J.H. Frederick, Multidimensional quantum dynamics with trajectories: a novel numerical implementation of Bohmian mechanics 332 (2000) 145
Nesbitt, D.J., see Harper, W.W. 335 (2001) 381
Neuendorf, R., R.E. Palmer and R. Smith, Low energy deposition of size-selected Si clusters onto graphite 333 (2001) 304
Neugebauer, H., see Miller, E.K. 335 (2001) 23
Neumark, D.M., see Liu, Z. 332 (2000) 65
Neumark, D.M., see Pivonka, N.L. 334 (2001) 24
Ng, C.Y., see Chen, Y.-J. 336 (2001) 105
Nguyen, M.T. and T.-K. Ha, Decomposition mechanism of the polynitrogen N_5 and N_6 clusters and their ions 335 (2001) 311

Nikolić, S., N. Trinajstić and M. Randić, Wiener index revisited 333 (2001) 319
Nishikawa, T., see Ishikawa, Y. 333 (2001) 199
Nishimura, S., see Kandori, H. 334 (2001) 271
Nishimura, Y., see Kanada, T. 332 (2000) 442
Nizkorodov, S.A., see Harper, W.W. 335 (2001) 381
Nogami, T., see Mito, M. 333 (2001) 69
Nogami, Y., see Terazima, M. 332 (2000) 503
Noid, D.W., see Gray, S.K. 333 (2001) 308
Nonn, T. and T. Plakhotnik, Fluorescence excitation spectroscopy of vibronic transitions in single molecules 336 (2001) 97
Nordholm, S., see Krems, R.V. 335 (2001) 273
Nordling, J., see Hinde, R.J. 339 (2001) 167
North, S.W., see Li, R. 334 (2001) 47
Novikov, E., N. Boens and J. Hofkens, New strategies for low light level detection in single molecule spectroscopy 338 (2001) 151
Novoderezhkin, V., A. Taisova and Z.G. Fetisova, Unit building block of the oligomeric chlorosomal antenna of the green photosynthetic bacterium *Chloroflexus aurantiacus*: modeling of nonlinear optical spectra 335 (2001) 234
Nugent, K.W., see Prawer, S. 332 (2000) 93

Obraztsova, E.D., see Simakin, A.V. 332 (2000) 231
O'Connell, M.J., see Walters, D.A. 338 (2001) 14
Oestreich, M., see Meskers, S.C.J. 339 (2001) 223
Ogata, A., see Einaga, H. 338 (2001) 303
Ogawa, T., see Ohno, K. 332 (2000) 167
Ohno, K., M. Yamazaki, N. Kishimoto, T. Ogawa and K. Takeshita, Trajectory calculations of two-dimensional Penning ionization electron spectra of N_2 in collision with metastable $He^* 2^3S$ atoms 332 (2000) 167
Ohshima, Y., see Egashira, K. 334 (2001) 285
Ohta, N., see Kanada, T. 332 (2000) 442
Ohtani, S., see Furuhashi, O. 337 (2001) 94
Ohtsuka, Y., see Sen, R. 332 (2000) 467
Okabe, T., M. Kawata, Y. Okamoto and M. Mikami, Replica-exchange Monte Carlo method for the isobaric–isothermal ensemble 335 (2001) 435
Okada, A. and H. Sumi, Vibrational energy accumulation in dendrimers by infrared radiation, inducing nonlinear dependence of isomerization rates on the low light intensity 340 (2001) 336
Okada, T., see Nakashima, S. 331 (2000) 396
Okamoto, Y., see Mitsutake, A. 332 (2000) 131
Okamoto, Y., see Ishikawa, Y. 333 (2001) 199
Okamoto, Y., see Okabe, T. 335 (2001) 435
Okazaki, I., Y. Hara and M. Nagaoka, On vibrational cooling upon photodissociation of carbonmonoxymyoglobin and its microscopic mechanism from the viewpoint of vibrational modes of heme 337 (2001) 151
Okazaki, N., see Chie, K. 334 (2001) 55
Okazaki, S., see Shinoda, K. 337 (2001) 306
Okotrub, A.V., see Kuznetsov, V.L. 336 (2001) 397
Ólafsson, A., see Peeters, R. 337 (2001) 231

Olejniczak, Z., see Birczyński, A. 339 (2001) 229
Oleynikov, N.N., see Davydov, V.A. 333 (2001) 224
Oliva, M., V.S. Safont, J. Andrés and O. Tapia, Electronic mechanistic pattern for C–C bond-breaking from transition structures in Rubisco's chemistry 340 (2001) 391
Oliva, R., see Lima, C.A.S. 332 (2000) 428
Oliveira Jr., O.N., see Cavalli, A. 338 (2001) 88
Oliveira, O.N., see Dynarowicz-atka, P. 337 (2001) 11
Oliveira, O.N., see Haas, H. 335 (2001) 510
Olszewski, R. and M. Zubek, A study of electron impact excitation of the $A^2\Sigma^+$ state of nitric oxide in the near-threshold energy range 340 (2001) 249
O'Malley, P.J., Density functional predicted geometries and vibrational frequencies of the neutral and anion-radical form of pheophytin: relevance to electron transfer in photosynthetic reaction centres 331 (2000) 78
Omi, H., see Nagasaka, B. 340 (2001) 473
Onishi, H., see Yamakata, A. 333 (2001) 271
Onishi, T., see Takano, Y. 335 (2001) 395
Oppel, M. and G.K. Paramonov, Optimal control of rotational motion of dissociation fragments by infrared laser pulses: application to a three-dimensional model of $HONO_2$ in the gas phase at temperatures below 1 K 339 (2001) 243
Orlando, R., see Baranek, Ph. 340 (2001) 362
Ornellas, F.R., Theoretical spectroscopic characterization of the $B^2\Sigma^+$ state of SiP and of the $X^2\Pi$–$B^2\Sigma^+$ and $A^2\Sigma^+$–$B^2\Sigma^+$ transitions 335 (2001) 420
Orr, B.J., see He, Y. 335 (2001) 215
Orr-Ewing, A.J., see Rudić, S. 332 (2000) 487
Orwa, J.O., see Prawer, S. 332 (2000) 93
Östmark, H., see Bittererová, M. 340 (2001) 597
Ostroverkhov, V., R.G. Petschek, K.D. Singer and R.J. Twieg, Λ-like chromophores for chiral non-linear optical materials 340 (2001) 109
Oswald, I.D.H., see Bourhill, G. 336 (2001) 234
Ota, T., see Miyasaka, H. 335 (2001) 496
Ottinger, Ch. and A. Kowalski, Hot-atom chemiluminescence: a beam study of the $N(^4S) + CH_4$ system 339 (2001) 53
Oweimreen, G.A. and J.S. Hwang, Evidence of tilt angle in an 8CB–10CB mixture 334 (2001) 83
Owenius, R., see Engström, M. 338 (2001) 407
Owrutsky, J.C., see Baronavski, A.P. 333 (2001) 36
Oya, M., see Shiina, H. 336 (2001) 242
Ozaki, Y., K. Horiai, T. Konno and H. Uehara, Infrared absorption spectroscopy of $Ar–^{12}C^{18}O_2$: change in the intramolecular potential upon complex formation 335 (2001) 188

Pålsson, L.O., see Bourhill, G. 336 (2001) 234
Paar, V., N. Pavin, A. Rubčić, J. Rubčić and N. Trinajstić, Scale-invariant power law and fractality for molecular weights 336 (2001) 129
Pace, I.D., see Pietraperzia, G. 335 (2001) 195
Pacios, L.F., see Gálvez, O. 337 (2001) 263
Packer, K.J., see Graham, R.G. 332 (2000) 319
Painelli, A., see Freo, L.D. 338 (2001) 208
Pal, S. and S. Prakash, Erratum to "Partial double- and single-differential cross-sections for CO_2 by electron collision" [Chem. Phys. Lett. 308 (1999) 428–436] 340 (2001) 612

Palmer, R.E., see Neuendorf, R. 333 (2001) 304
Palmqvist, A.E.C., see Baudin, M. 335 (2001) 517
Pan, C., see Yuan, L. 340 (2001) 237
Pan, J.S., see Guo, Y.P. 339 (2001) 319
Panek, J. and Z. Latajka, A theoretical study of NO_2 complexes with aluminium and gallium based on topological analysis of electron density and electron localization function 332 (2000) 617
Panja, S. and S. Chakravorti, "Dynamics of twisted intramolecular charge transfer process of 4-*N*, *N*-dimethylaminocinnamic acid in α-cyclodextrin environment" [Chem. Phys. Lett. 336 (2001) 57–62] 338 (2001) 217
Panja, S. and S. Chakravorti, Dynamics of twisted intramolecular charge transfer process of 4-N,N-dimethylaminocinnamic acid in α-cyclodextrin environment 336 (2001) 57
Pannier, M., see Jeschke, G. 331 (2000) 243
Panten, D., see Léonard, C. 335 (2001) 97
Papadimitrakopoulos, F., see Ispasoiu, R.G. 340 (2001) 7
Papp, J.G., see Torday, L.L. 334 (2001) 381
Parac, M., see Grimme, S. 334 (2001) 99
Paramonov, G.K., see Oppel, M. 339 (2001) 243
Park, J., see Bae, S.Y. 336 (2001) 219
Park, J., see Lee, C.J. 337 (2001) 398
Park, J., see Lee, C.J. 338 (2001) 113
Park, J., see Lee, C.J. 340 (2001) 413
Parneix, P., see Bréchignac, C. 335 (2001) 34
Parusel, A.B.J., Excited state intramolecular charge transfer in *N*,*N*-heterocyclic-4-aminobenzonitriles: a DFT study 340 (2001) 531
Paschek, D. and R. Krishna, Inter-relation between self- and jump-diffusivities in zeolites 333 (2001) 278
Pasqualini, E.E. and M. López, C_{11} linear chains and monocyclic rings 336 (2001) 33
Pasterny, K., see Gwóźdź, E. 335 (2001) 71
Pastirk, I., V.V. Lozovoy and M. Dantus, Femtosecond photon echo and virtual echo measurements of the vibronic and vibrational coherence relaxation times of iodine vapor 333 (2001) 76
Paszkowicz, W., see Iwanowski, R.J. 336 (2001) 226
Patchett, A.J., see Meißen, F. 336 (2001) 181
Pathak, R.K., see Kulkarni, S.A. 336 (2001) 278
Patzlaff, T., see Seifert, G. 333 (2001) 248
Pavin, N., see Paar, V. 336 (2001) 129
Payne, D.S., G.J. Wilson and R. Devonshire, Non-thermal nuclear hyperfine populations in the products of a photodissociation reaction 332 (2000) 58
Pecul, M., J. Lewandowski and J. Sadlej, Benchmark calculations of the shielding constants in the water dimer 333 (2001) 139
Pederson, M.R., see Kortus, J. 340 (2001) 565
Pedrini, C., see Guerassimova, N. 339 (2001) 197
Peeters, J., see Vereecken, L. 333 (2001) 162
Peeters, R., G. Berden, A. Ólafsson, L.J.J. Laarhoven and G. Meijer, Cavity enhanced absorption spectroscopy in the 10 μm region using a waveguide CO_2 laser 337 (2001) 231
Pejov, L., A gradient-corrected density functional study of indole self-association through N–H$\cdots\pi$ hydrogen bonding 339 (2001) 269

Pekker, S., see Fülöp, F. 334 (2001) 233
Peled, S., see Leu, G. 332 (2000) 344
Peng, H.Y., see Zhou, X.T. 332 (2000) 215
Peng, J.C., see Chen, X.H. 336 (2001) 201
Peng, J.L., see Prawer, S. 332 (2000) 93
Peng, X., X. Zhu, X. Fang, M. Feng, K. Gao, X. Yang and M. Liu, Preparation of pseudo-pure states by line-selective pulses in nuclear magnetic resonance 340 (2001) 509
Penke, B., see Torday, L.L. 334 (2001) 381
Pepi, F., see Cacace, F. 339 (2001) 71
Perczel, A., see Torday, L.L. 334 (2001) 381
Peremans, A., see Dreesen, L. 333 (2001) 327
Pereverzev, Y.V., O.V. Prezhdo and L.R. Dalton, Mean-field theory of acentric order of chromophores with displaced dipoles 340 (2001) 328
Pérez-Jiménez, A.J., J.M. Pérez-Jordá and J.C. Sancho-García, A DFT study of analytical correlated densities 331 (2000) 101
Pérez-Jordá, J.M., see Pérez-Jiménez, A.J. 331 (2000) 101
Pern, G.Y., see White, J.D. 338 (2001) 263
Pernot, P., see Heninger, M. 333 (2001) 358
Perrin, M.-Y., see Martin, J.-P. 332 (2000) 283
Persky, A., see Kornweitz, H. 331 (2000) 132
Petcu, S., see Ténégal, F. 335 (2001) 155
Peteanu, L.A., see Walters, K.A. 339 (2001) 255
Petelenz, B., see Birczyński, A. 339 (2001) 229
Petelenz, P., see Andrzejak, M. 332 (2000) 435
Petelenz, P., see Munn, R.W. 336 (2001) 357
Peterka, D.S., see Ahmed, M. 339 (2001) 203
Petrosyan, A.G., see Guerassimova, N. 339 (2001) 197
Petrukhin, A.N., see Antipin, S.A. 331 (2000) 378
Petschek, R.G., see Ostroverkhov, V. 340 (2001) 109
Peverall, R., see Barry, H.R. 333 (2001) 285
Peyerimhoff, S.D., see Hanrath, M. 337 (2001) 368
Peyerimhoff, S.D., see Mühlhäuser, M. 336 (2001) 171
Peyerimhoff, S.D., see Schnell, M. 340 (2001) 559
Phillips, D.L., see Cheng, Y.F. 338 (2001) 308
Piancastelli, M.N., see Hjelte, I. 334 (2001) 151
Picconatto, C.A., A. Srivastava and J.J. Valentini, State-to-state dynamics of the $H + CD_3(CH_2)_4CD_3 \rightarrow H_2 + CD_3((CH_2)_3CH)CD_3$ reaction: Dynamics of abstraction of secondary H in linear alkanes 340 (2001) 317
Pickard, C.J., see Winkler, B. 337 (2001) 36
Piecuch, P., see Kowalski, K. 334 (2001) 89
Piecuch, P., see Torday, L.L. 334 (2001) 381
Pierard, N., A. Fonseca, Z. Konya, I. Willems, G. Van Tendeloo and J.B. Nagy, Production of short carbon nanotubes with open tips by ball milling 335 (2001) 1
Pierloot, K., see Hasegawa, J.-y. 335 (2001) 503
Pietraperzia, G., M. Becucci, I.D. Pace, I. López-Tocón and E. Castellucci, Rotationally resolved electronic spectroscopy of aniline excited vibronic levels 335 (2001) 195
Pietrewicz, B.A., see Kisiel, Z. 333 (2001) 381

Pingale, S.S. and S.R. Gadre, Polarization-corrected molecular electrostatic potential for the cation binding problem 340 (2001) 604
Pino, T., Ph. Bréchignac, E. Dartois, K. Demyk and L. d'Hendecourt, Electronic spectroscopy of a cyclopentafused PAH cation, the fluorene$^+$: comparison between gas phase and matrix spectra 339 (2001) 64
Piris, J., see Wegewijs, B.R. 332 (2000) 79
Pis Diez, R. and J.A. Alonso, Theoretical evidence of bound metastable states in the doubly ionized nickel dimer Ni_2^{2+} 332 (2000) 481
Piskorz, W., see Brocławik, E. 333 (2001) 332
Pivonka, N.L., T. Lenzer, M.R. Furlanetto and D.M. Neumark, Photoelectron spectroscopy of Xe_nI^- clusters ($n \leqslant 13$) 334 (2001) 24
Plašil, R., see Glosík, J. 331 (2000) 209
Plakhotnik, T., see Nonn, T. 336 (2001) 97
Plaza, P., see Changenet-Barret, P. 336 (2001) 439
Pliego Jr. J.R. and J.M. Riveros, New values for the absolute solvation free energy of univalent ions in aqueous solution 332 (2000) 597
Podo, F., see Casieri, C. 338 (2001) 137
Pokorná, Z., see Juha, L. 335 (2001) 539
Polzonetti, G., V. Carravetta, A. Ferri, P. Altamura, M. Alagia, R. Richter and M.V. Russo, Photoelectron spectroscopy (PES) study of gas-phase 2,5-(2,2′-dithienyl)-diethynyl-thiophene (TRIM): an experimental and theoretical study 340 (2001) 449
Pommeret, S., see Jarzęba, W. 333 (2001) 419
Pompe, W., see Jost, O. 339 (2001) 297
Popov, A.A., see Dorozhko, P.A. 336 (2001) 39
Popov, A.M., see Lozovik, Yu.E. 335 (2001) 348
Popov, A.V. and N. Agmon, Three-dimensional simulation verifies theoretical asymptotics for reversible binding 340 (2001) 151
Porcher, P., see Albuquerque, R.Q. 331 (2000) 519
Porshnev, P.I., see Martin, J.-P. 332 (2000) 283
Poterya, V., see Glosík, J. 331 (2000) 209
Pouchan, C., M. Aouni and D. Bégué, Ab initio determination of the anharmonic vibrational spectra of P_2O in the region 200–2000 cm^{-1} 334 (2001) 352
Pouchan, C., see Mérawa, M. 334 (2001) 403
Pouillon, Y. and C. Massobrio, A density functional study of CuO_2 molecules: structural stability, bonding and temperature effects 331 (2000) 290
Poulsen, J., S.R. Keiding and P.J. Rossky, Extracting rates of vibrational energy relaxation from centroid molecular dynamics 336 (2001) 488
Pradeep, T., see Resmi, M.R. 333 (2001) 515
Pradeep, T., see Sandhyarani, N. 338 (2001) 33
Pradhan, B.K., see Adu, C.K.W. 337 (2001) 31
Prakash, S., see Pal, S. 340 (2001) 612
Pramada, K.P., see Jin, Z. 337 (2001) 43
Prato, M., see Kordatos, K. 334 (2001) 221
Pratt, D.W., see Hockridge, M.R. 334 (2001) 31
Prawer, S., K.W. Nugent, D.N. Jamieson, J.O. Orwa, L.A. Bursill and J.L. Peng, The Raman spectrum of nanocrystalline diamond 332 (2000) 93
Premvardhan, L.L., see Walters, K.A. 339 (2001) 255
Prezhdo, O.V., see Pereverzev, Y.V. 340 (2001) 328

Price, S.L., see van Mourik, T. 331 (2000) 253
Priyakumar, U.D., T.C. Dinadayalane and G. Narahari Sastry, Structures, energetics and vibrational spectra of the valence isomers of phosphinine. An ab initio and DFT study 336 (2001) 343
Priyakumar, U.D., T.C. Dinadayalane and G.N. Sastry, An ab initio and DFT study of the valence isomers of pyridine 337 (2001) 361
Pronina, O.P., see Davydov, V.A. 333 (2001) 224
Pszczółkowski, L., see Kisiel, Z. 333 (2001) 381
Pullerits, T., see Grage, M.M.-L. 339 (2001) 96
Pullerits, T., see He, Z. 334 (2001) 159
Puranik, M., J. Chandrasekhar and S. Umapathy, Structure of the triplet excited state of tetrabromo-*p*-benzoquinone from time-resolved resonance Raman spectra and ab initio calculations 337 (2001) 224
Purtov, P.A., see Fedin, M.V. 339 (2001) 395

Qian, C.X.W., see Ding, C.-F. 331 (2000) 163
Qin, X.C., see Walters, D.A. 338 (2001) 14
Qiu, J., A.L. Gaeta and K. Hirao, Long-lasting phosphorescence in oxygen-deficient Ge-doped silica glasses at room temperature 333 (2001) 236
Qu, Z.-w., H. Zhu, Z.-s. Li and Q.-y. Zhang, Theoretical study on the mechanism of the reaction: $HCCCH_2^+ + C_2H_2 \rightarrow c\text{-}C_3H_3^+ + C_2H_2$ 336 (2001) 325
Qu, Z.-w., H. Zhu, Z.-s. Li and Q.-y. Zhang, Theoretical study on the reaction mechanism of BH_2^+ and ethylene in gas-phase 339 (2001) 140
Quiñonero, D., A. Frontera, P. Ballester, C. Garau, A. Costa and P.M. Deyà, A topological analysis of charge density in complexes between derivatives of squaric acid and ammonium cation 339 (2001) 369

Rada, T., see Bitzer, T. 331 (2000) 433
Radloff, W., see Stert, V. 337 (2001) 299
Raghunath, P., see Vivekananda, S. 332 (2000) 251
Rahman, S., see Claye, A. 333 (2001) 16
Rahn, M.D., see Buckley, A.R. 339 (2001) 331
Raina, G. and G.U. Kulkarni, A molecular beam study of water–methanol clusters 337 (2001) 269
Raju, A.R., see Sudheendra, L. 340 (2001) 275
Rakhmanina, A.V., see Davydov, V.A. 333 (2001) 224
Rakov, N., C.B. de Araújo, G.B. da Rocha, A.M. Simas, P.A.F. Athayde-Filho and J. Miller, Two-photon absorption in mesoionic compounds pumped at the visible and at the infrared 332 (2000) 13
Ramírez, R., see Böhm, M.C. 332 (2000) 117
Ramachandran, B., N. Balakrishnan and A. Dalgarno, Vibrational–rotational distributions of NO formed from $N + O_2$ reactive collisions 332 (2000) 562
Ramaekers, R., see Dkhissi, A. 331 (2000) 553
Ramanathan, K.V., see Sinha, N. 332 (2000) 125
Ran, Q., see Shi, Q. 339 (2001) 154
Rana, D. and G. Gangopadhyay, Steady-state spectral properties of dendrimer supermolecule as a light harvesting system 334 (2001) 314
Randić, M., see Nikolić, S. 333 (2001) 319
Rao, C.N.R., see Murugavel, P. 331 (2000) 149
Räsänen, M.O., see Firsov, D.A. 338 (2001) 317

Rashin, A.A., I.A. Topol, G.J. Tawa and S.K. Burt, Charge distributions in water and ion–water clusters 335 (2001) 327
Rasmussen, A.J., S.J. Jeffrey and S.C. Smith, Subspace wavepacket evolution with Newton polynomials 336 (2001) 149
Rasmusson, M., A.N. Tarnovsky, E. Åkesson and V. Sundström, On the use of two-photon absorption for determination of femtosecond pump–probe cross-correlation functions 335 (2001) 201
Rassolov, V.A., see Garashchuk, S. 333 (2001) 459
Rastogi, R.C., see Jain, S.K. 331 (2000) 547
Raupp-Kossmann, R.A. and C. Scharnagl, pK_a shifts for protonation-dependent degrees of freedom 336 (2001) 177
Rayane, D., see Dugourd, P. 336 (2001) 511
Rayez, J.C., see Bonnet, L. 338 (2001) 385
Re, N., see Cerofolini, G.F. 333 (2001) 181
Re, N., see Cerofolini, G.F. 339 (2001) 375
Rebane, A., see Drobizhev, M. 334 (2001) 76
Reddy, B.V., S.N. Khanna and S.C. Deevi, Electronic structure and magnetism in $(FeAl)_n (n \leqslant 6)$ clusters 333 (2001) 465
Redlich, Ph., see Seeger, T. 339 (2001) 41
Redondo, C., M.N. Sánchez Rayo, J.A. Fernández, D. Husain and F. Castaño, Collisionally induced intramultiplet mixing of $Sr(5^3P_J)$ metastable states by Ne, Kr and Xe atoms 331 (2000) 365
Redondo, P., C. Barrientos and A. Largo, Structures and stabilities of MgC_3 isomers: a theoretical study 335 (2001) 64
Regan, P., see Ahmed, M. 339 (2001) 203
Reich, A., see Möschel, C. 335 (2001) 9
Reid, S.A., see Su, H. 335 (2001) 17
Reinhardt, W.P., see Miller, M.A. 331 (2000) 278
Rejto, P.A., see Verkhivker, G.M. 336 (2001) 495
Rejto, P.A., see Verkhivker, G.M. 337 (2001) 181
Rekhi, S., see Dubrovinsky, L.S. 333 (2001) 264
Remko, M., O.A. Walsh and W.G. Richards, Ab initio and DFT study of molecular structure and tautomerism of 2-amino-2-imidazoline, 2-amino-2-oxazoline and 2-amino-2-thiazoline 336 (2001) 156
Ren, Y., K.-i. Iimura and T. Kato, Monodispersed two-dimensional nanoclusters of $CF_3(CF_2)_3(CH_2)_{22}COOH$ on the aqueous Cd^{2+} subphase investigated by polarization modulation infrared spectroscopy 332 (2000) 339
Ren, Z.F., see Li, W.Z. 335 (2001) 141
Renn, A., see Segura, J.-M. 340 (2001) 77
Renou, F. and M. Mostafavi, Reactivity of the solvated electron toward divalent magnesium 335 (2001) 363
Rérat, M., see Mérawa, M. 334 (2001) 403
Resmi, M.R., S. Ma, R. Caprioli and T. Pradeep, $C_{120}O_n$ from $C_{60}Br_{24}$ 333 (2001) 515
Rey, R., see Llanta, E. 340 (2001) 173
Reynaud, C., see Ténégal, F. 335 (2001) 155
Reynolds, D., see Lewis, E.K. 334 (2001) 357
Ricca, A., see Walch, S.P. 333 (2001) 6
Ricci, A., see de Petris, G. 332 (2000) 290

Ricci, A., see Di Stefano, G. 331 (2000) 196
Rice, J.H., J.-P. Galaup, N. Wachter, P.R. Birkett and R. Taylor, Fluorescence and phosphorescence of $C_{70}Ph_{10}$ and $C_{70}Cl_{10}$ in toluene between 5 and 300 K 335 (2001) 553
Rice, J.H., see Schwell, M. 339 (2001) 29
Richard, A., see Azoulay, J. 331 (2000) 347
Richards, W.G., see Remko, M. 336 (2001) 156
Richardson, N.V., see Bitzer, T. 331 (2000) 433
Richardson, S.L., see Kortus, J. 340 (2001) 565
Richter, R., see Polzonetti, G. 340 (2001) 449
Riganelli, A., see Varandas, A.J.C. 331 (2000) 331
Righi, A., see Bendiab, N. 339 (2001) 305
Ritchie, G.A.D., see Barry, H.R. 333 (2001) 285
Ritze, H.-H., see Stert, V. 337 (2001) 299
Rius i Riu, J., A. Karawajczyk, M. Stankiewicz, K. Yoshiki Franzén, P. Winiarczyk and L. Veseth, Non-Franck–Condon effects in the photoionization of molecular oxygen to the O_2^+ X $^2\Pi_g$ state in the 19–31 eV photon energy region 333 (2001) 91
Rius i Riu, J., A. Karawajczyk, M. Stankiewicz, K. Yoshiki Franzén, P. Winiarczyk and L. Veseth, Non Franck–Condon effects in the photoionization of molecular nitrogen to the $N_2^+A^2\Pi_u$ state in the 19–34 eV photon energy region 338 (2001) 285
Riveros, J.M., see J.R. Pliego Jr., 332 (2000) 597
Robertson, E.G., see Hockridge, M.R. 334 (2001) 31
Rocca, M., see Vattuone, L. 331 (2000) 177
Rocha, A.B. and C.E. Bielschowsky, Intensity of the n $\rightarrow \pi^*$ symmetry-forbidden electronic transition in acetone by direct vibronic coupling mechanism 337 (2001) 331
Rocha, G.B., see Albuquerque, R.Q. 331 (2000) 519
Rocha, W.R., K. Coutinho, W.B. de Almeida and S. Canuto, An efficient quantum mechanical/molecular mechanics Monte Carlo simulation of liquid water 335 (2001) 127
Rockenbauer, A., see Fülöp, F. 334 (2001) 233
Rode, M., J. Sadlej, R. Moszynski, P.E.S. Wormer and A. van der Avoird, Reply to the Comment on "The importance of high-order correlation effects for the CO–CO interaction potential" [Chem. Phys. Lett. 314 (1999) 326] 334 (2001) 424
Rodriguez, A., E. Garcia, A. Ceballos and A. Laganà, A trajectory study of the OH+H_2 reaction 333 (2001) 471
Rodriguez, J.A., J. Hrbek, J. Dvorak, T. Jirsak and A. Maiti, Interaction of sulfur with TiO_2(110): photoemission and density-functional studies 336 (2001) 377
Rodríguez-Santiago, L., O. Vendrell, I. Tejero, M. Sodupe and J. Bertran, Solvent-assisted catalysis in the enolization of acetaldehyde radical cation 334 (2001) 112
Rogers, D.M., see Bramwell, M.J. 331 (2000) 483
Rogers, K.M., P.W. Fowler and G. Seifert, Chemical versus steric frustration in boron nitride heterofullerene polyhedra 332 (2000) 43
Rolim, F., J.P. Braga and J.R. Mohallem, Unified description of chemical bonding in H_2 isotopomers, including Ps_2, μ_2 and bi-excitons 332 (2000) 139
Romanenko, A.I., see Kuznetsov, V.L. 336 (2001) 397
Romero, H.E., see Adu, C.K.W. 337 (2001) 31
Roos, B.O., see Gagliardi, L. 331 (2000) 229
Roos, B.O., see Hasegawa, J.-y. 335 (2001) 503
Ros, T.D., see Kordatos, K. 334 (2001) 221

Rosca, F., D. Ionascu, A.T.N. Kumar, A.A. Demidov and P.M. Champion, Femtosecond coherence spectroscopy using spectrally selective differential photodetection 337 (2001) 107
Rose, P.W., see Verkhivker, G.M. 336 (2001) 495
Rose, P.W., see Verkhivker, G.M. 337 (2001) 181
Rosemeyer, M., R. Schäfer and J.A. Becker, Acceleration of neutral silicon cluster isomers in a helium gas expansion 339 (2001) 323
Rosmus, P., see Cours, T. 331 (2000) 317
Rosmus, P., see Léonard, C. 335 (2001) 97
Rossi, M., see Terranova, M.L. 336 (2001) 405
Rossky, P.J., see Poulsen, J. 336 (2001) 488
Rotger, M., V. Boudon, H. Bürger and H. Willner, High-resolution spectroscopy and analysis of the ν_4 band of $^{80}SeF_6$ 339 (2001) 83
Rout, C., see Jain, S.K. 331 (2000) 547
Rowat, T.E., see Gough, T.E. 333 (2001) 230
Royen, P., see Derkatch, A. 332 (2000) 278
Rozas, I., see Espinosa, E. 336 (2001) 457
Rozenbaum, V.M., see Mebel, A.M. 336 (2001) 135
Rubčić, A., see Paar, V. 336 (2001) 129
Rubčić, J., see Paar, V. 336 (2001) 129
Rudić, S., D. Ascenzi and A.J. Orr-Ewing, Rotational distribution of the HCl products from the reaction of $Cl(^2P)$ atoms with methanol 332 (2000) 487
Rühle, M., see Mayne, M. 338 (2001) 101
Rühle, M., see Seeger, T. 339 (2001) 41
Ruike, M., see Iiyama, T. 331 (2000) 359
Runge, K., see Henderson, T.M. 337 (2001) 138
Ruseckas, A., see Grage, M.M.-L. 339 (2001) 96
Ruseckas, A., see Theander, M. 337 (2001) 277
Rusli., see Gan, B. 333 (2001) 23
Russo, M.V., see Polzonetti, G. 340 (2001) 449
Rutigliano, M., M. Cacciatore and G.D. Billing, Hydrogen atom recombination on graphite at 10 K via the Eley–Rideal mechanism 340 (2001) 13
Rutter, M.D., R.A. Secco and Y. Huang, Ionic conduction in hydrated zeolite Li-, Na- and K-A at high pressures 331 (2000) 189
Ruud, K., P.R. Taylor and P.-O. Åstrand, Zero-point vibrational effects on optical rotation 337 (2001) 217
Ruud, K., see Jaszuński, M. 336 (2001) 473

Sadlej, A.J., see Turski, P. 338 (2001) 345
Sadlej, J., Theoretical study of structure and spectra of cage clusters $(H_2O)_n$, n=11,12 333 (2001) 485
Sadlej, J., see Pecul, M. 333 (2001) 139
Sadlej, J., see Rode, M. 334 (2001) 424
Saeki, M., T. Tsukuda and T. Nagata, Ab initio study of $(CO_2)_n^-$: structures and stabilities of isomers 340 (2001) 376
Saenger, W., E.B. Starikov, K. Bräsicke and E.W. Knapp, Negative solubility coefficient of methylated cyclodextrins in water: A theoretical study 336 (2001) 504
Safont, V.S., see Oliva, M. 340 (2001) 391

Saga, N., Y. Kimura, N. Hirota and M. Terazima, Photo-thermalization processes of charge transfer complexes in liquids studied by the transient grating method 332 (2000) 496
Sage, I.C., see Bourhill, G. 336 (2001) 234
Sahin, C., see Adam, W. 340 (2001) 26
Saigusa, H. and E.C. Lim, Picosecond photodissociation study of the excimer formation in van der Waals dimers of aromatic molecules 336 (2001) 65
Saito, K., see Takahashi, O. 338 (2001) 398
Saito, K., see Yuan, L. 340 (2001) 237
Saito, T., see Fuji, T. 332 (2000) 324
Saito, Y. and H.-o. Hamaguchi, Dynamic symmetry lowering of the sulfate ion in aqueous solution probed by polarization-resolved CARS spectroscopy 339 (2001) 351
Sakai, M., M. Ichida and A. Nakamura, Raman scattering study of photopolymerization kinetics in C_{60} crystals 335 (2001) 559
Sakakibara, Y., see Vacha, M. 331 (2000) 387
Sakamoto, K., see Ideue, S. 337 (2001) 79
Sakisato, N., see Inaba, A. 340 (2001) 400
Sala, F.D., H.H. Heinze and A. Görling, Excitation energies of terthiophene and its dioxide derivative: a first-principles study 339 (2001) 343
Salaneck, W.R., see Luo, Y. 337 (2001) 176
Samuel, I.D.W., see Bourhill, G. 336 (2001) 234
Sánchez Rayo, M.N., see Redondo, C. 331 (2000) 365
Sánchez-Obregón, R., see García-Jiménez, F. 331 (2000) 42
Sancho-García, J.C., see Pérez-Jiménez, A.J. 331 (2000) 101
Sandhyarani, N. and T. Pradeep, Oxidation of alkanethiol monolayers on gold cluster surfaces 338 (2001) 33
Sankar, G., see Bromley, S.T. 340 (2001) 524
Santoro, G., see Serra, S. 331 (2000) 339
Sapre, A.V., see Naik, P.D. 340 (2001) 116
Sarasola, C., J.E. Fowler, J.M. Elorza and J.M. Ugalde, On the critical stability of dipole bound dianions 337 (2001) 355
Sariciftci, S., see Brabec, C.J. 340 (2001) 232
Sarkisov, O.M., see Antipin, S.A. 331 (2000) 378
Sastry, G.N., see Priyakumar, U.D. 337 (2001) 361
Sastry, M.D., see Bhide, M.K. 332 (2000) 98
Sato, M., see Nakashima, S. 331 (2000) 396
Sato, T., see Ma, R. 337 (2001) 61
Sauerwein, R.A. and S. Kais, Quantum critical phenomena in the Schrödinger formulation: mapping to classical lattices 333 (2001) 451
Sauge, S., P. Valiron and I. Mayer, Dissociative recombination of antiprotonic atomcules $\bar{p}He^+$ with positronium: towards antihydrogen synthesis? 334 (2001) 330
Sauvajol, J.L., see Bendiab, N. 339 (2001) 305
Savio, L., see Vattuone, L. 331 (2000) 177
Savitsky, A.N., M. Galander and K. Möbius, W-band time-resolved electron paramagnetic resonance spectroscopy on transient organic radicals in solution 340 (2001) 458
Saxena, A., see Tretiak, S. 331 (2000) 561
Saxena, S.K., see Dubrovinsky, L.S. 333 (2001) 264
Sayós, R., see González, M. 335 (2001) 339

Saykally, R.J., see Michael, E.A. 338 (2001) 277
Scalas, E., see Haas, H. 335 (2001) 510
Scalmani, G., see Improta, R. 336 (2001) 349
Scandolo, S., see Serra, S. 331 (2000) 339
Schön, J.H., see Frolov, S.V. 334 (2001) 65
Schäfer, R., see Rosemeyer, M. 339 (2001) 323
Schaefer III, H.F., see Ignatyev, I.S. 337 (2001) 158
Schaefer III, H.F., see Ignatyev, I.S. 337 (2001) 169
Schall, M., see Walther, M. 332 (2000) 389
Schanne-Klein, M.C., F. Hache, T. Brotin, C. Andraud and A. Collet, Magnetic chiroptical effects in surface second harmonic reflection 338 (2001) 159
Schanne-Klein, M.C., see Mesnil, H. 338 (2001) 269
Schanze, K.S., see Walters, K.A. 339 (2001) 255
Scharnagl, C., see Raupp-Kossmann, R.A. 336 (2001) 177
Schermann, J.P., see Carles, S. 334 (2001) 374
Schinke, R. and M. Bittererová, On the $S_1 \rightarrow S_0$ internal conversion in the photodissociation of HNCO: the role of the NC stretch as a promoting mode 332 (2000) 611
Schlegel, H.B., see Cross, J.B. 340 (2001) 343
Schlegel, H.B., see Halls, M.D. 339 (2001) 427
Schmidt, K., see Agranovich, V.M. 336 (2001) 536
Schmitt, U., see Heid, M. 334 (2001) 119
Schnell, I. and A. Watts, Towards selective recoupling and mutual decoupling of dipolar-coupled spin pairs in double-quantum magic-angle spinning NMR experiments on multiply labelled solid-state samples 335 (2001) 111
Schnell, M., M. Mühlhäuser, G.E. Froudakis and S.D. Peyerimhoff, Ab initio CCSD(T) and MRD-CI study of excited states and the electronic spectrum of linear C_5^+ 340 (2001) 559
Schoonman, J., see Goossens, A. 331 (2000) 1
Schromm, S., see Waldmann, O. 332 (2000) 73
Schulte, J., see Böhm, M.C. 332 (2000) 117
Schulz, J.J. and R. Koch, Scanning tunneling microscope controlled diffusion on Ag(110) 331 (2000) 119
Schwartz, D.A., see Boulet, A.M. 331 (2000) 108
Schweig, A., see Langenscheidt, A. 331 (2000) 203
Schwell, M., N.K. Wachter, J.H. Rice, J.-P. Galaup, S. Leach, R. Taylor and R.V. Bensasson, Coupling a dendrimer and a fullerene chromophore: a study of excited state properties of C_{61}(poly(aryl)acetylene)$_2$ 339 (2001) 29
Scuseria, G.E., see Bettinger, H.F. 332 (2000) 35
Secco, R.A., see Rutter, M.D. 331 (2000) 189
Seccombe, D.P., R.P. Tuckett, H.-W. Jochims and H. Baumgärtel, The observation of fluorescence from excited states of NF_2 and NF following the photodissociation of NF_3 in the 11–30 eV range 339 (2001) 405
Seeger, T., Ph. Redlich, N. Grobert, M. Terrones, D.R.M. Walton, H.W. Kroto and M. Rühle, SiO_x-coating of carbon nanotubes at room temperature 339 (2001) 41
Segawa, Y., see Zeng, H. 331 (2000) 71
Segawa, Y., see Zeng, H. 338 (2001) 241
Segura, J.-M., G. Zumofen, A. Renn, B. Hecht and U.P. Wild, Tip-induced spectral dynamics of single molecules 340 (2001) 77

Seifert, G., see Rogers, K.M. 332 (2000) 43
Seifert, G., T. Patzlaff and H. Graener, Ultrafast vibrational dynamics of doubly hydrogen bonded acetic acid dimers in liquid solution 333 (2001) 248
Seike, K., see Nakashima, S. 331 (2000) 396
Seikh, Md.M., see Sudheendra, L. 340 (2001) 275
Seki, K., Y. Sumiyoshi and Y. Endo, Rotational spectrum of the Kr–HCO^+ ionic complex 331 (2000) 184
Sekkat, Z., see Hayazawa, N. 335 (2001) 369
Sen, K.D., see Nagy, Á. 332 (2000) 154
Sen, P.N., see Leu, G. 332 (2000) 344
Sen, R., A. Govindaraj, K. Suenaga, S. Suzuki, H. Kataura, S. Iijima and Y. Achiba, Encapsulated and hollow closed-cage structures of WS_2 and MoS_2 prepared by laser ablation at 450–1050°C 340 (2001) 242
Sen, R., Y. Ohtsuka, T. Ishigaki, D. Kasuya, S. Suzuki, H. Kataura and Y. Achiba, Time period for the growth of single-wall carbon nanotubes in the laser ablation process: evidence from gas dynamic studies and time resolved imaging 332 (2000) 467
Senyavin, V.M., see Davydov, V.A. 333 (2001) 224
Senyavin, V.M., see Dorozhko, P.A. 336 (2001) 39
Seo, Y., Y. Kim and Y. Kim, MC-QCISD calculations for proton affinities of molecules and geometries 340 (2001) 186
Sepaniak, M.J., see Hinde, R.J. 339 (2001) 167
Sepaniak, M.J., see Lavrik, N.V. 336 (2001) 371
Sera, K., see Judai, K. 334 (2001) 277
Serdar Sariciftci, N., see Miller, E.K. 335 (2001) 23
Serra, S., S. Iarlori, E. Tosatti, S. Scandolo and G. Santoro, Dynamical and thermal properties of polyethylene by ab initio simulation 331 (2000) 339
Sessa, V., see Terranova, M.L. 336 (2001) 405
Seta, P., see Koudoumas, E. 335 (2001) 533
Sett, P., S. Chattopadhyay and P.K. Mallick, Excited state molecular configuration of biphenyl 331 (2000) 215
Seybold, P.G., see Kreye, W.C. 335 (2001) 257
Sha, G., see Sun, M. 339 (2001) 413
Shafeev, G.A., see Simakin, A.V. 332 (2000) 231
Shaik, S., see Filatov, M. 332 (2000) 409
Shang, N.G., see Zhou, X.T. 332 (2000) 215
Shen, D., see Yu, G. 333 (2001) 207
Shen, G., see Dubrovinsky, L.S. 333 (2001) 264
Shen, X. and J.R. Knutson, Femtosecond internal conversion and reorientation of 5-methoxyindole in hexadecane 339 (2001) 191
Shen, X., see Fang, L. 332 (2000) 299
Shen, Y., see Murata, H. 339 (2001) 161
Shen, Z., I. Boustani, M. Erdmann and V. Engel, Characterization of nuclear wave packets prepared by chirped femtosecond pulses using time-resolved photoelectron spectroscopy 339 (2001) 362
Sheng, L.-S., see He, T.-J. 332 (2000) 545
Sheng, Z., see Zhou, X. 339 (2001) 117
Sheu, W.-S., see Chen, H.-Y. 335 (2001) 475
Shi, C., see Su, H. 335 (2001) 17

Shi, Q., Q. Ran, W.S. Tam, J.W-H. Leung and A.S-C. Cheung, Laser-induced fluorescence spectroscopy of CrS 339 (2001) 154
Shi, Z., see Li, Y. 337 (2001) 403
Shi, Z., Y. Li, S. Wang, Z. Guo, C. Du, S. Xiao, N. Sun, Y. Cao, J. Yao, D. Zhu, E. Gao and S. Cai, Self-assembled film of a new C_{60} derivative covalently linked to TiO_2 nanocrystalline 336 (2001) 19
Shiau, C.-W., see Churikov, V.M. 332 (2000) 19
Shibata, Y., see Kandori, H. 334 (2001) 271
Shichida, Y., see Kandori, H. 334 (2001) 271
Shiga, M., M. Tachikawa and S. Miura, Ab initio molecular orbital calculation considering the quantum mechanical effect of nuclei by path integral molecular dynamics 332 (2000) 396
Shiina, H., K. Tsuchiya, M. Oya, A. Miyoshi and H. Matsui, Reaction rates of $O(^3P)$ atom with fluoroethanes at 1000–1400 K 336 (2001) 242
Shiliang, Q., see Song, Y. 338 (2001) 108
Shimizu, A. and H. Tachikawa, The dynamics on migrations of Li^+ ion and Li atom at 700 K around the circumference of graphite cluster model: A direct molecular dynamics study 339 (2001) 110
Shimizu, O., J. Watanabe and S. Naito, Transient near-IR absorption spectrum in laser flash photolyzed aqueous solutions of tris(2,2′-bipyridyl) ruthenium(II) 332 (2000) 295
Shingaya, Y. and M. Ito, Temperature dependence of adlayers on Pt(111) and Au(111) in a sulfuric acid solution studied by in situ IRAS 340 (2001) 425
Shinoda, K., S. Miura and S. Okazaki, Isotope effect on the structure of quantum fluid: a generalized Ornstein–Zernike analysis 337 (2001) 306
Shinoda, W. and M. Mikami, Self-guided molecular dynamics in the isothermal–isobaric ensemble 335 (2001) 265
Shinohara, H., see Hino, S. 337 (2001) 65
Shiomi, Y., see Karantonis, A. 335 (2001) 221
Shiyanovskii, S.V., see Smalyukh, I.I. 336 (2001) 88
Shoute, L.C.T., K.J. Falk and R.P. Steer, Spectroscopy and photophysics of 5-nitrotropolone in condensed media 332 (2000) 359
Shoute, L.C.T., S. Hirayama and R.P. Steer, Vibronically selective intersystem crossing in van der Waals complexes of 9-cyanoanthracene with xenon 338 (2001) 123
Shub, B.R., see Buchachenko, A.L. 340 (2001) 103
Siatecki, Z., see Jaszewski, A.R. 331 (2000) 403
Siebbeles, L.D.A., see van der Horst, J.-W. 334 (2001) 303
Siebrand, W. and M.Z. Zgierski, Theoretical study of the structure of phenol–ammonia complexes subject to proton transfer 334 (2001) 127
Silva Filho, D.A., see Dynarowicz-atka, P. 337 (2001) 11
Silvi, B., see Calatayud, M. 333 (2001) 493
Simakin, A.V., E.D. Obraztsova and G.A. Shafeev, Laser-induced carbon deposition from supercritical benzene 332 (2000) 231
Simas, A.M., see Hallwass, F. 335 (2001) 43
Simas, A.M., see Rakov, N. 332 (2000) 13
Simon, F., see Fülöp, F. 334 (2001) 233
Simons, J., see Skurski, P. 337 (2001) 143
Simons, J.P., see Hockridge, M.R. 334 (2001) 31
Sims, I.R., see Chastaing, D. 331 (2000) 170

Singel, D.J., see Boulet, A.M. 331 (2000) 108
Singer, K.D., see Ostroverkhov, V. 340 (2001) 109
Singer, S., see Leu, G. 332 (2000) 344
Singhal, R.P., see Tzallas, P. 332 (2000) 236
Sinha, A.K., D.W. Hwang and L.-P. Hwang, A novel approach to bulk synthesis of carbon nanotubes filled with metal by a catalytic chemical vapor deposition method 332 (2000) 455
Sinha, N. and K.V. Ramanathan, Use of polarization inversion for resolution of small dipolar couplings in SLF-2D NMR experiments – an application to liquid crystals 332 (2000) 125
Sinisterra, R.D., see Marques-Netto, A. 333 (2001) 371
Sirenko, A., see Claye, A. 333 (2001) 16
Skodje, R.T., see Chao, S.D. 336 (2001) 364
Skokov, S., see Zou, S. 339 (2001) 290
Skurski, P., M. Gutowski, R. Barrios and J. Simons, Non-ionic and zwitterionic forms of neutral arginine – an ab initio study 337 (2001) 143
Sloop, D.J., see Yang, T.-C. 331 (2000) 489
Slovokhotov, Y., see Iida, S. 338 (2001) 21
Smalley, R.E., see Walters, D.A. 338 (2001) 14
Smaiyukh, I.I., S.V. Shiyanovskii and O.D. Lavrentovich, Three-dimensional imaging of orientational order by fluorescence confocal polarizing microscopy 336 (2001) 88
Smith, B.W., D.E. Luzzi and Y. Achiba, Tumbling atoms and evidence for charge transfer in $La_2@C_{80}@SWNT$ 331 (2000) 137
Smith, G.D., see Borodin, O. 336 (2001) 292
Smith, I.W.M., see Chastaing, D. 331 (2000) 170
Smith, K., see Walters, D.A. 338 (2001) 14
Smith, R., see Neuendorf, R. 333 (2001) 304
Smith, S.C., see Rasmussen, A.J. 336 (2001) 149
So, C.R., see Bauschlicher, C.W. 333 (2001) 1
Socaciu, L.D., J. Hagen, U. Heiz, T.M. Bernhardt, T. Leisner and L. Wöste, Reaction mechanism for the oxidation of free silver dimers 340 (2001) 282
Sodupe, M., see Rodríguez-Santiago, L. 334 (2001) 112
Softley, T.P., see Dickinson, H. 338 (2001) 37
Softley, T.P., see Monti, O.L.A. 333 (2001) 146
Soldán, P., see Lee, E.P.F. 336 (2001) 479
Soldatović, T., see Gutman, I. 334 (2001) 168
Someda, K., see Takahashi, S. 335 (2001) 241
Son, K.H., see Lee, C.J. 338 (2001) 113
Song, K. and M.A. Collins, A classical trajectory study of sym-triazine photodissociation on an interpolated potential energy surface 335 (2001) 481
Song, W.H., see Wu, X.C. 336 (2001) 53
Song, Y., Q. Shiliang, W. Yuxiao, Q. Zhang and X. Xin, Excited state optical nonlinearity of inorganic metal cluster $WSe_4(AgPPh_3)_3Cl$ with picosecond pulses 338 (2001) 108
Song, Y., see Li, Y. 337 (2001) 403
Sood, A.K., see Murugavel, P. 331 (2000) 149
Sordo, J.A., see Valdés, H. 333 (2001) 169
Sorensen, S.L., see Hjelte, I. 334 (2001) 151
Sosa, C., see Cremer, D. 337 (2001) 199

Spano, F.C., Emission from aggregates of oligo-phenylene vinylenes: a recipe for superradiant *H*-aggregates 331 (2000) 7
Spichiger, D., G. Carver, C. Dobe, J. Bendix, P.L.W. Tregenna-Piggott, R. Meier and G. Zahn, Electronic Raman transitions from the vanadium(III) hexa-aqua cation, in guanidinium vanadium sulphate 337 (2001) 391
Spiess, H.W., see Jeschke, G. 331 (2000) 243
Sprengers, J.P., see Bazalgette Courrèges-Lacoste, G. 335 (2001) 209
Springborg, M., Poly(cyanoacetylene): a conjugated polymer with a rich phase diagram 339 (2001) 389
Srinivas, R., see Vivekananda, S. 332 (2000) 251
Srivastava, A., see Picconatto, C.A. 340 (2001) 317
Stafström, S., L. Hultman and N. Hellgren, Predicted stability of a new aza[60]fullerene molecule, $C_{48}N_{12}$ 340 (2001) 227
Stagira, S., see Cerullo, G. 335 (2001) 27
Stair, P.C., see Briggman, K.A. 334 (2001) 1
Staker, W.S., see Becerra, R. 333 (2001) 83
Stankiewicz, M., see Rius i Riu, J. 333 (2001) 91
Stankiewicz, M., see Rius i Riu, J. 338 (2001) 285
Starikov, E.B., see Saenger, W. 336 (2001) 504
Staroverov, V.N. and E.R. Davidson, A density functional method for degenerate spin-multiplet components 340 (2001) 142
Steer, R.P., see Shoute, L.C.T. 332 (2000) 359
Steer, R.P., see Shoute, L.C.T. 338 (2001) 123
Steffen, M., see Chang, D.E. 338 (2001) 337
Stepanek, I., G. Maurin, P. Bernier, J. Gavillet, A. Loiseau, R. Edwards and O. Jaschinski, Nano-mechanical cutting and opening of single wall carbon nanotubes 331 (2000) 125
Stephan, O., see Mittal, J. 339 (2001) 311
Stert, V., P. Farmanara, H.-H. Ritze, W. Radloff, K. Gasmi and A. Gonzalez-Ureña, Femtosecond time-resolved electron spectroscopy of the intracluster reaction in Ba $\cdots FCH_3$ 337 (2001) 299
Stickel, R.E., see Estupiñán, E.G. 336 (2001) 109
Stickland, R.J., see Bentley, J. 332 (2000) 85
Stoch, G., see Birczyński, A. 339 (2001) 229
Stolte, S., see Bazalgette Courrèges-Lacoste, G. 335 (2001) 209
Stręk, W., see Dereń, P.J. 332 (2000) 308
Strekalov, M.L., Evaluation of the contribution of elastic dephasing processes in linewidths 332 (2000) 525
Streltsov, A.I., see Dobrodey, N.V. 339 (2001) 263
Strizhak, P.E., see Didenko, O.Z. 340 (2001) 55
Strohkendl, F.P., R.J. Larsen, L.R. Dalton and Z.K. Kafafi, Femtosecond nearly degenerate four-wave mixing in C_{60} films between 0.55 and 0.70 μm 331 (2000) 354
Strokach, Yu.P., see Antipin, S.A. 331 (2000) 378
Su, H., Z. Jia, C. Shi, J. Xin and S.A. Reid, Study of energy transfer in $KMgF_3$:Eu–X (X=Gd, Cr, Ce) by the decay model of $^6P_{7/2}$ exited state of Eu^{2+} 335 (2001) 17
Su, M.-D., see Lin, C.-L. 339 (2001) 147
Su, P.-H. and C.-S. Yeh, Photofragmentation of the Ag^+–furan complex in the gas-phase 331 (2000) 420
Subramanian, V., see Amutha, R. 335 (2001) 489

Sudheendra, L., Md.M. Seikh, A.R. Raju and C. Narayana, An infrared spectroscopic study of the low-spin to intermediate-spin state ($^1A_1$–$^3T_1$) transition in rare earth cobaltates, $LnCoO_3$ (Ln = La, Pr and Nd) 340 (2001) 275
Suematsu, H., see Fujiwara, A. 336 (2001) 205
Suenaga, K., see Sen, R. 340 (2001) 242
Suenram, R.D., see McIntosh, A. 331 (2000) 95
Sugiki, S.-I., see Kitaura, K. 336 (2001) 163
Sugita, Y., see Ishikawa, Y. 333 (2001) 199
Sugita, A., K. Suto, M. Kawasaki and Y. Matsumi, Controlling the branching ratio of the photodissociation of aligned Cl_2 at 404 nm 340 (2001) 83
Sugny, D. and M. Joyeux, A new canonical perturbation procedure for studying nonadiabatic dynamics 337 (2001) 319
Sui, Y., D. Wang, J. Yin, Z.-k. Zhu and Z.-g. Wang, Investigation of dipole orientation in a side-chain second-order nonlinear optical poly(urethane-imide) by real-time variable temperature FT-IR spectroscopy 339 (2001) 186
Suits, A.G., see Ahmed, M. 339 (2001) 203
Sultan, R. and R. Halabieh, Effect of an electric field on propagating $Co(OH)_2$ Liesegang patterns 332 (2000) 331
Sumanasekera, G.U., see Adu, C.K.W. 337 (2001) 31
Sumanasekera, G.U., see Claye, A. 333 (2001) 16
Sumi, H., see Okada, A. 340 (2001) 336
Sumiyoshi, Y., see Seki, K. 331 (2000) 184
Sumpter, B.G., see Gray, S.K. 333 (2001) 308
Sun, F., G.P. Glass and R.F. Curl, The photolysis of NO_2 at 193 nm 337 (2001) 72
Sun, H., see Jung, J. 336 (2001) 311
Sun, J.-L., see Li, Y.-M. 338 (2001) 297
Sun, L.F., Z.Q. Liu, X.C. Ma, D.S. Tang, W.Y. Zhou, X.P. Zou, Y.B. Li, J.Y. Lin, K.L. Tan and S.S. Xie, Growth of carbon nanofibers array under magnetic force by chemical vapor deposition 336 (2001) 392
Sun, L.F., Z.Q. Liu, X.C. Ma, Z.Y. Zhong, S.B. Tang, Z.T. Xiong, D.S. Tang, W.Y. Zhou, X.P. Zou, Y.B. Li, K.L. Tan, S.S. Xie and J.Y. Lin, Growth of carbon nanotube arrays using the existing array as a substrate and their Raman characterization 340 (2001) 222
Sun, M., G. Sha, S. Cong, F. Ma, J. Xie and C. Zhang, Collisional quantum interference effect on rotational energy transfer in an atom–diatom system 339 (2001) 413
Sun, N., see Shi, Z. 336 (2001) 19
Sun. Q., see Wang, Y. 334 (2001) 411
Sun, X.H., see Liao, L.S. 333 (2001) 212
Sun, Y.P., see Wu, X.C. 336 (2001) 53
Sun, Z., see Wang, J. 340 (2001) 98
Sun, Z., see Zeng, H. 338 (2001) 241
Sundström, V., see He, Z. 334 (2001) 159
Sundström, V., see Rasmusson, M. 335 (2001) 201
Sundström, V., see Theander, M. 337 (2001) 277
Sundström, V., see Grage, M.M.-L. 339 (2001) 96
Suresh, D., see Hanf, A. 340 (2001) 71
Suryaprakash, N., see Vivekanandan, S. 338 (2001) 247
Suto, K., see Sugita, A. 340 (2001) 83
Suzuki, A., see Tsushima, S. 334 (2001) 365

Suzuki, S., see Fujiwara, A. 336 (2001) 205
Suzuki, S., see Sen, R. 332 (2000) 467
Suzuki, S., see Sen, R. 340 (2001) 242
Suzuki, Y., Raman spectroscopic study of hyperquenched glassy water in the presence of different non-ionic solutes 335 (2001) 357
Svensson, M., see Theander, M. 337 (2001) 277
Svensson, S., see Hjelte, I. 334 (2001) 151
Svensson, T., see Nelander, B. 332 (2000) 403
Svensson, T., see Nelander, B. 339 (2001) 295
Svishchev, I.M., see Zasetsky, A.Yu. 334 (2001) 107
Symons, M.C.R., Comment on "Raman spectra of low- and high-density amorphous ices" [Chem. Phys. Lett. 293 (1998) 412] 333 (2001) 322
Syvitski, R.T., see Burnell, E.E. 331 (2000) 455
Szafrański, M., see Katrusiak, A. 340 (2001) 302
Szwarc, H., see Davydov, V.A. 333 (2001) 224

Tabak, M., see Haas, H. 335 (2001) 510
Tachibana, M., K. Kojima, R. Ikuyama, Y. Kobayashi and M. Ataka, Sound velocity and dynamic elastic constants of lysozyme single crystals 332 (2000) 259
Tachikawa, H. and T. Yamano, Ab initio MO calculations of hyperfine coupling constants of hydronium radical H_3O 335 (2001) 305
Tachikawa, H., see Shimizu, A. 339 (2001) 110
Tachikawa, M., see Shiga, M. 332 (2000) 396
Taday, P.F., see Tzallas, P. 332 (2000) 236
Tafazzoli, M. and S. Jalili, Absolute partition coefficients for organic solutes by using Monte Carlo simulations in chloroform/water system 331 (2000) 235
Tai, Y. and J. Murakami, Surface-induced fragmentation of tin cluster ions on a highly oriented pyrolytic graphite surface 339 (2001) 9
Taisova, A., see Novoderezhkin, V. 335 (2001) 234
Takabayashi, Y., see Iida, S. 338 (2001) 21
Takabayashi, Y., see Kubozono, Y. 335 (2001) 163
Takada, T., H. Koizumi, T. Ichikawa and A. Lund, Photoinduced isomerization of alkyl radicals in low-temperature solids: dependence of its efficiency on the position of the radical site 335 (2001) 375
Takada, T., see Koizumi, H. 340 (2001) 256
Takahashi, K., see Kasuya, D. 337 (2001) 25
Takahashi, K., see Kokai, F. 332 (2000) 449
Takahashi, K., see Murata, K. 331 (2000) 14
Takahashi, O., N. Kurushima, A. Kawano and K. Saito, Possibility of the magnetic field effect on the thermal decomposition of N_2O : molecular dynamics simulation 338 (2001) 398
Takahashi, S. and K. Someda, Classical irregular scattering and fluctuation of quantum transition probability 335 (2001) 241
Takano, Y., S. Kubo, T. Onishi, H. Isobe, Y. Yoshioka and K. Yamaguchi, Theoretical studies on the magnetic interaction and reversible dioxygen binding of the active site in hemocyanin 335 (2001) 395
Takayanagi, T. and A. Wada, Theoretical calculations for the prereaction processes of the D···HF and H···DF van der Waals molecules 338 (2001) 195
Takechi, M., see Yoshida, N. 332 (2000) 265

Takeda, K., see Mito, M. 333 (2001) 69
Takei, S., see Vacha, M. 331 (2000) 387
Takeshita, K., see Ohno, K. 332 (2000) 167
Taketsugu, T. and S. Carter, A variational determination of spin-rovibronic energy levels of MgNC in the $A^2\Pi$ state 340 (2001) 385
Taketsugu, T., see Kumeda, Y. 333 (2001) 29
Takizawa, M., see Bandow, S. 337 (2001) 48
Taleb-Bendiab, A. and D. Chomiak, Millimeter-wave spectrum of MgSH 334 (2001) 195
Taliani, C., see Munn, R.W. 336 (2001) 357
Tam, W.S., see Shi, Q. 339 (2001) 154
Tamai, N., see Yang, X. 334 (2001) 257
Tan, K.L., see Sun, L.F. 336 (2001) 392
Tan, K.L., see Sun, L.F. 340 (2001) 222
Tang, B.-Y., see Chen, M.-D. 337 (2001) 349
Tang, C.C., S.S. Fan, M.L. de la Chapelle and P. Li, Silica-assisted catalytic growth of oxide and nitride nanowires 333 (2001) 12
Tang, D., see Liu, Y. 331 (2000) 31
Tang, D.S., see Sun, L.F. 336 (2001) 392
Tang, D.S., see Sun, L.F. 340 (2001) 222
Tang, S.B., see Sun, L.F. 340 (2001) 222
Tang, X.J., see Lei, H. 333 (2001) 387
Tang, X.-W., see Leu, G. 332 (2000) 344
Tang, Z.K., see Wang, N. 339 (2001) 47
Tani, T., see Vacha, M. 331 (2000) 387
Tanimoto, Y., see Chie, K. 334 (2001) 55
Tanizaki, M., see Hoshi, N. 336 (2001) 13
Tapia, O., see Oliva, Mó. 340 (2001) 391
Tappero, R., P. Wolfers and A. Lichanot, Electronic, magnetic structures and neutron diffraction in B_1 and B_3 phases of MnS: a density functional approach 335 (2001) 449
Tarnovsky, A.N., see Rasmusson, M. 335 (2001) 201
Tawa, G.J., see Rashin, A.A. 335 (2001) 327
Taylor, P.R., see Ruud, K. 337 (2001) 217
Taylor, R., see Rice, J.H. 335 (2001) 553
Taylor, R., see Schwell, M. 339 (2001) 29
Tchénio, P., see Azoulay, J. 331 (2000) 347
Teixeira, P.I.C., see Cleaver, D.J. 338 (2001) 1
Tejero, I., see Rodríguez-Santiago, L. 334 (2001) 112
Ténégal, F., S. Petcu, N. Herlin-Boime, X. Armand, M. Mayne and C. Reynaud, Effect of the C/O ratio on the C_{60} and C_{70} formation rates in soot synthesised by laser pyrolysis of benzene-based mixtures 335 (2001) 155
Teodoro, O.M.N., see Lourenço, J.M.C. 336 (2001) 431
ter Meulen, J.J., see van Beek, M.C. 337 (2001) 237
Terazima, M., see Saga, N. 332 (2000) 496
Terazima, M., Y. Nogami and T. Tominaga, Diffusion of a radical from an initiator of a free radical polymerization: a radical from AIBN 332 (2000) 503
Terlouw, J.K., see Vivekananda, S. 332 (2000) 251
Terranova, M.L., V. Sessa and M. Rossi, Tree-like carbon nanostructures generated by the action of atomic hydrogen on glassy carbon 336 (2001) 405

Terrones, M., see Mayne, M. 338 (2001) 101
Terrones, M., see Seeger, T. 339 (2001) 41
Theander, M., M. Svensson, A. Ruseckas, D. Zigmantas, V. Sundström, M.R. Andersson and O. Inganäs, High luminescence from a substituted polythiophene in a solvent with low solubility 337 (2001) 277
Theander, M., see Grage, M.M.-L. 339 (2001) 96
Thimm, G., see Winkler, B. 337 (2001) 36
Thiry, P.A., see Dreesen, L. 333 (2001) 327
Tho Nguyen, M., see Delaere, D. 333 (2001) 103
Thomas, J.M., see Bromley, S.T. 340 (2001) 524
Thompson, D.E., K.A. Merchant and M.D. Fayer, Solute–solvent interactions: two-dimensional ultrafast infrared vibrational echo experiments 340 (2001) 267
Thompson, L.K., see Waldmann, O. 332 (2000) 73
Tian, A., see Wang, X. 338 (2001) 367
Tian, Y.J., see He, J.L. 340 (2001) 431
Tian, Y.J., see Wang, T.S. 334 (2001) 7
Tichý, M., see Glosík, J. 331 (2000) 209
Ticich, T.M., see Vander Wal, R.L. 336 (2001) 24
Tikhonov, G., see Kasperovich, V. 337 (2001) 55
Timmel, C.R., F. Cintolesi, B. Brocklehurst and P.J. Hore, Model calculations of magnetic field effects on the recombination reactions of radicals with anisotropic hyperfine interactions 334 (2001) 387
Tipple, C.A., see Lavrik, N.V. 336 (2001) 371
Titman, J.J., see Heindrichs, A.S.D. 335 (2001) 89
Titov, A.A., see Antipin, S.A. 331 (2000) 378
Tohdoh, A. and K. Kaneko, Effect of coadsorbed CO_2 on the magnetic properties of O_2 confined in graphitic slit-shaped micropores 340 (2001) 33
Tokura, S., see Zeng, H. 331 (2000) 71
Tomikawa, K., see Kanno, H. 333 (2001) 324
Tominaga, T., see Terazima, M. 332 (2000) 503
Tominaga, Y., see Amo, Y. 332 (2000) 521
Toniolo, A., see Magnier, S. 338 (2001) 329
Topol, I.A., see Rashin, A.A. 335 (2001) 327
Topp, M.R., see Chen, Y. 337 (2001) 284
Torchet, G., see van de Waal, B.W. 331 (2000) 57
Torday, L.L., R. Burcl, A.K. Füzéry, P. Császár, O. Farkas, A. Perczel, M.A. Zamora, J.G. Papp, B. Penke, P. Piecuch and I.G. Csizmadia, Can NO_2^+ exist in bent or cyclic forms? 334 (2001) 381
Torres, L., M. Moreno and J.M. Lluch, A discrete variable representation study of the dynamics of the double proton transfer in bicyclic oxalamidines 340 (2001) 591
Tortajada, J., see Boutreau, L. 338 (2001) 74
Tosatti, E., see Serra, S. 331 (2000) 339
Toulhoat, P., see Boutreau, L. 338 (2001) 74
Tozer, D.J., see Wilson, P.J. 337 (2001) 341
Tregenna-Piggott, P.L.W., see Spichiger, D. 337 (2001) 391
Tretiak, S., A. Saxena, R.L. Martin and A.R. Bishop, CEO/semiempirical calculations of UV–visible spectra in conjugated molecules 331 (2000) 561
Trikoupis, M.A., see Vivekananda, S. 332 (2000) 251

Trinajstić, N., see Nikolić, S. 333 (2001) 319
Trinajstić, N., see Paar, V. 336 (2001) 129
Trofimov, A.V., see Adam, W. 340 (2001) 26
Trombetti, A., see Cané, E. 340 (2001) 356
Tsuchiya, K., see Shiina, H. 336 (2001) 242
Tsukuda, T., see Saeki, M. 340 (2001) 376
Tsushima, S., T. Yang and A. Suzuki, Theoretical Gibbs free energy study on $UO_2(H_2O)_n^{2+}$ and its hydrolysis products 334 (2001) 365
Tuckett, R.P., see Seccombe, D.P. 339 (2001) 405
Tunega, D., see Benco, L. 333 (2001) 479
Tung, C.H., see Lei, H. 333 (2001) 387
Turchanin, A., D. Nattland and W. Freyland, Surface freezing in a liquid eutectic Ga–Bi alloy 337 (2001) 5
Turski, P. and A.J. Sadlej, The change of picture contribution to relativistic corrections to second-order properties 338 (2001) 345
Tutti, F., see Dubrovinsky, L.S. 333 (2001) 264
Twieg, R.J., see Ostroverkhov, V. 340 (2001) 109
Tyuterev, V.G., see Cours, T. 331 (2000) 317
Tyutyulkov, N., F. Dietz and K. Müllen, Magnetic exchange interaction between π-electron radicals adsorbed on α-boron-nitride surfaces 331 (2000) 465
Tzallas, P., C. Kosmidis, P. Graham, K.W.D. Ledingham, T. McCanny, S.M. Hankin, R.P. Singhal, P.F. Taday and A.J. Langley, Coulomb explosion in aromatic molecules and their deuterated derivatives 332 (2000) 236
Tzeli, D., A. Mavridis and S.S. Xantheas, A molecular level study of the aqueous microsolvation of acetylene 340 (2001) 538

Uchida, M., see Murata, H. 339 (2001) 161
Uchimaru, T., see Chandra, A.K. 334 (2001) 200
Uebayasi, M., see Kitaura, K. 336 (2001) 163
Uehara, H., see Ozaki, Y. 335 (2001) 188
Ugalde, J.M., see Sarasola, C. 337 (2001) 355
Ujiie, T., see Ito, T. 340 (2001) 308
Umapathy, S., see Puranik, M. 337 (2001) 224
Umecky, T., see Kanakubo, M. 338 (2001) 95
Umishita, K., see Hino, S. 337 (2001) 65
Unni Nair, B., see Amutha, R. 335 (2001) 489
Upadhyaya, H.P., see Naik, P.D. 340 (2001) 116

Vacha, M., S. Takei, K.-i. Hashizume, Y. Sakakibara and T. Tani, Onset of exciton–polariton behavior observed in individual fibers of pseudoisocyanine J-aggregates by sub-micron scale reflectance spectroscopy 331 (2000) 387
Vahtras, O., see Engström, M. 338 (2001) 407
Valbusa, U., see Vattuone, L. 331 (2000) 177
Valdés, H. and J.A. Sordo, The pentamethylene sulfide · · · HCl dimer: a theoretical study 333 (2001) 169
Valentini, J.J., see Picconatto, C.A. 340 (2001) 317

Valiron, P., see Sauge, S. 334 (2001) 330
van Beek, M.C. and J.J. ter Meulen, An intense pulsed electrical discharge source for OH molecular beams 337 (2001) 237
van de Waal, B.W., G. Torchet and M.-F. de Feraudy, Structure of large argon clusters Ar_N, $10^3 < N < 10^5$: experiments and simulations 331 (2000) 57
van der Avoird, A., see Rode, M. 334 (2001) 424
van der Horst, J.-W., P.A. Bobbert, P.H.L. de Jong, M.A.J. Michels, L.D.A. Siebbeles, J.M. Warman, G.H. Gelinck and G. Brocks, Predicting polarizabilities and lifetimes of excitons on conjugated polymer chains 334 (2001) 303
van der Zanden, B., see Goossens, A. 331 (2000) 1
van Erp, T.S. and E.J. Meijer, Hydration of methanol in water. A DFT-based molecular dynamics study 333 (2001) 290
van Faassen, E.E., see Kerp, H.R. 332 (2000) 5
van Gunsteren, W.F., see Walser, R. 334 (2001) 337
Van Guyse, M., see Cotlet, M. 336 (2001) 415
van Heijnsbergen, D., see von Helden, G. 333 (2001) 350
van Mourik, T., S.L. Price and D.C. Clary, Ab initio calculations on indole–water, 1-methylindole–water and indole–$(water)_2$ 331 (2000) 253
Van Tendeloo, G., see Pierard, N. 335 (2001) 1
Vander Wal, R.L. and T.M. Ticich, Comparative flame and furnace synthesis of single-walled carbon nanotubes 336 (2001) 24
Vanderleyden, J., see Cotlet, M. 336 (2001) 415
Vandersypen, L.M.K., see Chang, D.E. 338 (2001) 337
Vanquickenborne, L.G., see Delaere, D. 333 (2001) 103
Van-Quynh, A., see Korb, J.-P. 339 (2001) 77
Varandas, A.J.C. and L. Zhang, $OH(v) + O_3$: Does chemical reaction dominate over non-reactive quenching? 340 (2001) 62
Varandas, A.J.C. and L. Zhang, Test studies on the potential energy surface and rate constant for the $OH+O_3$ atmospheric reaction 331 (2000) 474
Varandas, A.J.C. and P.J.S.B. Caridade, The $OH(v') + O_2(v'')$ reaction: a new source of stratospheric ozone? 339 (2001) 1
Varandas, A.J.C., A.I. Voronin and I. Borges, On the interaction of two conical intersections: the H_6 system 331 (2000) 285
Varandas, A.J.C., A.I. Voronin, P.J.S.B. Caridade and A. Riganelli, Is there a barrier for the C_{2v} insertion reaction in $O(^1D)+H_2$? A test dynamics study based on two-valued energy-switching potential energy surfaces 331 (2000) 331
Varandas, A.J.C., see Yu, H.G. 334 (2001) 173
Vatsa, R.K. and H.-R. Volpp, Absorption cross-sections for some atmospherically important molecules at the H atom Lyman-α wavelength (121.567 nm) 340 (2001) 289
Vattuone, L., L. Savio, U. Valbusa and M. Rocca, Switching from molecular to dissociative adsorption with vibrational energy: ethylene on Ag(001) 331 (2000) 177
Vázquez, S.A., see Martínez-Núñez, E. 332 (2000) 583
Vendrell, O., see Rodríguez-Santiago, L. 334 (2001) 112
Vereecken, L. and J. Peeters, H-atom abstraction by OH-radicals from (biogenic) (poly)alkenes: C–H bond strengths and abstraction rates 333 (2001) 162

Verkhivker, G.M., P.A. Rejto, D. Bouzida, S. Arthurs, A.B. Colson, S.T. Freer, D.K. Gehlhaar, V. Larson, B.A. Luty, T. Marrone and P.W. Rose, Navigating ligand–protein binding free energy landscapes: universality and diversity of protein folding and molecular recognition mechanisms 336 (2001) 495
Verkhivker, G.M., P.A. Rejto, D. Bouzida, S. Arthurs, A.B. Colson, S.T. Freer, D.K. Gehlhaar, V. Larson, B.A. Luty, T. Marrone and P.W. Rose, Parallel simulated tempering dynamics of ligand–protein binding with ensembles of protein conformations 337 (2001) 181
Veseth, L., see Rius i Riu, J. 333 (2001) 91
Veseth, L., see Rius i Riu, J. 338 (2001) 285
Vila, A. and R.A. Mosquera, A comparative AIM study of alkyl monoethers and their protonated forms 332 (2000) 474
Villaeys, A.A., K.K. Liang and S.H. Lin, Influence of the transverse velocity on TC-RFWM spectra of jet-cooled CH 336 (2001) 268
Villard, B., see Bréchignac, C. 335 (2001) 34
Villarreal, P., see González-Lezana, T. 335 (2001) 105
Virgili, T., see Cerullo, G. 335 (2001) 27
Vitorge, P. and M. Masella, A theoretical study of $[Be_x(H_2O)_n]^{2+}$, $[BeOH_x(H_2O)_{n-1}]^{+}$ and $[Be(OH)_{2x}(H_2O)_{n-2}]$ aggregates (n=1–6). Incidence of the first hydration shells on the hydrolysis reactions of Be^{2+} and $BeOH^{+}$ systems 332 (2000) 367
Vivekananda, S., P. Raghunath, K. Bhanuprakash, R. Srinivas, M.A. Trikoupis and J.K. Terlouw, Characterization of iminothiosulfine-type ions $[HNCS_2]^{+/-}$ and their neutral counterparts by mass spectrometry and computational chemistry 332 (2000) 251
Vivekanandan, S. and N. Suryaprakash, Novel method of estimating proton–proton dipolar couplings to aid the analyses of NMR spectra of oriented molecules using two-dimensional inverse experiment 338 (2001) 247
Vogler, A., see Kunkely, H. 338 (2001) 29
Volkov, V.V., Z.L. Wang and B.S. Zou, Carrier recombination in clusters of NiO 337 (2001) 117
Volodin, A.M., K.A. Dubkov and A. Lund, Direct ESR detection of S = 3/2 states for nitrosyl iron complexes in FeZSM-5 zeolites 333 (2001) 41
Volpp, H.-R., see Hanf, A. 340 (2001) 71
Volpp, H.-R., see Vatsa, R.K. 340 (2001) 289
von Helden, G., D. van Heijnsbergen, M.A. Duncan and G. Meijer, IR-REMPI of vanadium-carbide nanocrystals: Ideal versus truncated lattices 333 (2001) 350
von Ragué Schleyer, P., see Ignatyev, I.S. 337 (2001) 158
von Ragué Schleyer, P., see Ignatyev, I.S. 337 (2001) 169
Voronin, A.I., see Varandas, A.J.C. 331 (2000) 285
Voronin, A.I., see Varandas, A.J.C. 331 (2000) 331
Vosch, T., see Hofkens, J. 333 (2001) 255
Vuković, S., see Gutman, I. 334 (2001) 168

Wachter, N., see Rice, J.H. 335 (2001) 553
Wachter, N.K., see Schwell, M. 339 (2001) 29
Wada, A., see Takayanagi, T. 338 (2001) 195
Wagner, D.R., see Michael, E.A. 338 (2001) 277
Waiblinger, M., see Goedde, B. 334 (2001) 12
Wakahara, T., see Kubozono, Y. 335 (2001) 163

Wakasa, M. and H. Hayashi, Can an external magnetic field affect the thermal reaction of pentafluorobenzyl chloride with *n*-butyllithium in hexane? 340 (2001) 493
Walch, S.P., C.W. Bauschlicher, A. Ricca and E.L.O. Bakes, On the reaction $CH_2O+NH_3 \rightarrow CH_2NH+H_2O$ 333 (2001) 6
Waldmann, O., R. Koch, S. Schromm, P. Müller, L. Zhao and L.K. Thompson, Magnetic anisotropy of a supramolecular Cu(II) [3 × 3] grid 332 (2000) 73
Waletzke, M., see Grimme, S. 334 (2001) 99
Wallace, M.I., see Ying, L. 334 (2001) 145
Walser, R., B. Hess, A.E. Mark and W.F. van Gunsteren, Further investigation on the validity of Stokes–Einstein behaviour at the molecular level 334 (2001) 337
Walsh, O.A., see Remko, M. 336 (2001) 156
Walsh, R., see Becerra, R. 333 (2001) 83
Walter, E.D., see Boulet, A.M. 331 (2000) 108
Walters, D.A., M.J. Casavant, X.C. Qin, C.B. Huffman, P.J. Boul, L.M. Ericson, E.H. Haroz, M.J. O'Connell, K. Smith, D.T. Colbert and R.E. Smalley, In-plane-aligned membranes of carbon nanotubes 338 (2001) 14
Walters, K.A., L.L. Premvardhan, Y. Liu, L.A. Peteanu and K.S. Schanze, Metal-to-ligand charge transfer absorption in a rhenium(I) complex that contains a π-conjugated bipyridine acceptor ligand 339 (2001) 255
Walther, M., B. Fischer, M. Schall, H. Helm and P.U. Jepsen, Far-infrared vibrational spectra of all-*trans*, 9-*cis* and 13-*cis* retinal measured by THz time-domain spectroscopy 332 (2000) 389
Walton, D.R.M., see Mayne, M. 338 (2001) 101
Walton, D.R.M., see Seeger, T. 339 (2001) 41
Wang, C., see Wang, X. 339 (2001) 36
Wang, D., see Sui, Y. 339 (2001) 186
Wang, D., see Wang, J. 340 (2001) 98
Wang, D., see Zalyubovsky, S.J. 335 (2001) 298
Wang, D.Z., see Li, W.Z. 335 (2001) 141
Wang, G.Z., see Wang, Y.W. 339 (2001) 174
Wang, H., see Hjelte, I. 334 (2001) 151
Wang, H.Z., see Lei, H. 333 (2001) 387
Wang, J., Light-induced pattern formation in the excitable Belousov–Zhabotinsky medium 339 (2001) 357
Wang, J., Photo-induced excitations in the ruthenium-catalyzed Belousov–Zhabotinsky reaction 335 (2001) 123
Wang, J., Z. Sun, X. Zhu, M. Ge and D. Wang, First experimental observation on different ionic states of the CH_3CH_2O radical: a HeI photoelectron spectrum of the ethoxy CH_3CH_2O radical 340 (2001) 98
Wang, J.N., see Cheng, J. 333 (2001) 375
Wang, J.X., see Chen, X.H. 336 (2001) 201
Wang, K.Y., see Wu, X.C. 336 (2001) 53
Wang, L., see Zhang, F. 337 (2001) 125
Wang, L., see Zhang, F. 337 (2001) 131
Wang, N., G.D. Li and Z.K. Tang, Mono-sized and single-walled 4 Å carbon nanotubes 339 (2001) 47
Wang, N., see Zhou, X.T. 332 (2000) 215

Wang, P., S. Zhang, P. Wu, C. Ye, H. Liu and F. Xi, Optical limiting properties of optically active phthalocyanine derivatives 340 (2001) 261
Wang, S. and G.C. Bazan, Exciplex formation with distyrylbenzene derivatives and *N,N*-dimethylaniline 333 (2001) 437
Wang, S., see Cheng, J. 333 (2001) 375
Wang, S., see Li, C. 340 (2001) 444
Wang, S., see Li, Y. 337 (2001) 403
Wang, S., see Shi, Z. 336 (2001) 19
Wang, T.S., D.L. Yu, Y.J. Tian, F.R. Xiao, J.L. He, D.C. Li, W.K. Wang and L. Li, Cubic-C_3N_4 nanoparticles synthesized in CN_x/TiN_x multilayer films 334 (2001) 7
Wang, T.S., see He, J.L. 340 (2001) 431
Wang, T.Y., see Gough, T.E. 333 (2001) 230
Wang, W.K., see Wang, T.S. 334 (2001) 7
Wang, X., A. Tian, N.B Wong, C.-K. Law and W.-K. Li, A Gaussian-3 investigation of N_7 isomers 338 (2001) 367
Wang, X., see Li, Y. 333 (2001) 153
Wang, X., see Liu, Y. 331 (2000) 31
Wang, X., Y. Liu and D. Zhu, Controlled growth of well-aligned carbon nanotubes with large diameters 340 (2001) 419
Wang, X., Z. Wang, Y. Liu, C. Wang, C. Bai and D. Zhu, Ring formation and fracture of a carbon nanotube 339 (2001) 36
Wang, X.-G., see Lin, H. 332 (2000) 569
Wang, Y., C.L. Hendrickson and A.G. Marshall, Direct optical spectroscopy of gas-phase molecular ions trapped and mass-selected by ion cyclotron resonance: laser-induced fluorescence excitation spectrum of hexafluorobenzene ($C_6F_6^+$) 334 (2001) 69
Wang, Y., Q. Sun, K. Fan and J. Deng, Interaction of halogen atom with Ag(110): ab initio pseudopotential density functional study 334 (2001) 411
Wang, Y.F., X.W. Cao, S.F. Hu, Y.Y. Liu and G.X. Lan, Graphical method for assigning Raman peaks of radial breathing modes of single-wall carbon nanotubes 336 (2001) 47
Wang, Y.W., G.W. Meng, C.H. Liang, G.Z. Wang and L.D. Zhang, Magnetic properties of ordered Fe_xAg_{1-x} nanowire arrays embedded in anodic alumina membranes 339 (2001) 174
Wang, Z., see Wang, X. 339 (2001) 36
Wang, Z.-g., see Sui, Y. 339 (2001) 186
Wang, Z.H., Y. Cao and G.Q. Xu, The binding of benzene on Si(111)-(7×7) : a theoretical modelling approach 338 (2001) 7
Wang, Z.L., see Volkov, V.V. 337 (2001) 117
Warman, J.M., see van der Horst, J.-W. 334 (2001) 303
Warman, J.M., see Wegewijs, B.R. 332 (2000) 79
Watanabe, J., see Shimizu, O. 332 (2000) 295
Watanabe, J., Y. Watanabe and S. Kinoshita, Relation between Stokes and anti-Stokes low-frequency light scattering in liquid carbon disulfide 333 (2001) 113
Watanabe, Y. and S. Kinoshita, Direct measurement of the frequency response function by means of frequency-domain four-wave mixing spectroscopy (FD-4WM) 331 (2000) 413
Watanabe, Y., see Watanabe, J. 333 (2001) 113
Watanabe, Y., see Zhang, J.-P. 331 (2000) 154
Watanabe, Y., see Zhang, J.-P. 332 (2000) 351
Watanabe, Y., see Zhang, J.-P. 340 (2001) 484

Watts, A., see Schnell, I. 335 (2001) 111
Webb, S.P., see Iordanov, T. 338 (2001) 389
Weber, J.M., J. Kim, E.A. Woronowicz, G.H. Weddle, I. Becker, O. Cheshnovsky and M.A. Johnson, Observation of resonant two-photon photodetachment of water cluster anions via femtosecond photoelectron spectroscopy 339 (2001) 337
Weddle, G.H., see Weber, J.M. 339 (2001) 337
Wee, A.T.S., see Guo, Y.P. 339 (2001) 319
Wegewijs, B.R., G. Dicker, J. Piris, A.A. García, M.P. de Haas and J.M. Warman, Photoelectron emission from conjugated polymer films: a potential source of artifacts in photoconductivity studies 332 (2000) 79
Wei, B., see Cao, A. 335 (2001) 150
Wei, Z.C., see Lei, H. 333 (2001) 387
Weiden, N., see Goedde, B. 334 (2001) 12
Weidinger, A., see Goedde, B. 334 (2001) 12
Weil, T., see Hofkens, J. 333 (2001) 255
Weiner, B.R., see Han, J. 332 (2000) 243
Weis, J.-J. and D. Levesque, Thermodynamic and structural properties of size-asymmetric charged hard spheres 336 (2001) 523
Weiser, P.S., see Wild, D.A. 332 (2000) 531
Weiss, G.H., see Berezhkovskii, A.M. 336 (2001) 321
Weiss, K., see Wöll, Ch. 332 (2000) 553
Weissman, S.I., see Yang, T.-C. 331 (2000) 489
Weitz, E., see Briggman, K.A. 334 (2001) 1
Weitzel, K.-M., see Korolkov, M.V. 336 (2001) 303
Wen, G.H., see Zhang, X.X. 333 (2001) 509
Wen, J.G., see Li, W.Z. 335 (2001) 141
Wermuth, M., see Heer, S. 334 (2001) 293
Wheatley, R.J., see Domene, C. 333 (2001) 403
White, J.D., J.H. Hsu, W.S. Fann, S.-C. Yang, G.Y. Pern and S.A. Chen, Deduction of the conformation of short chain luminescent conjugated polymers from single molecule photophysics 338 (2001) 263
Whitehead, J.C., see Bramwell, M.J. 331 (2000) 483
Whittaker, T.A., see Goedert, R.V. 332 (2000) 225
Wiesner, K., see Hjelte, I. 334 (2001) 151
Wild, D.A., Z.M. Loh, P.P. Wolynec, P.S. Weiser and E.J. Bieske, The Cl^-–CH_4 anion dimer: mid infrared spectrum and ab initio calculations 332 (2000) 531
Wild, U.P., see Segura, J.-M. 340 (2001) 77
Willems, I., see Pierard, N. 335 (2001) 1
Williams, F.A., see Yuan, L. 340 (2001) 237
Williart, A., see García, G. 335 (2001) 227
Willner, H., see Rotger, M. 339 (2001) 83
Wilson, C.C., Hydrogen atoms in acetylsalicylic acid (Aspirin): the librating methyl group and probing the potential well in the hydrogen-bonded dimer 335 (2001) 57
Wilson, G.J., see Payne, D.S. 332 (2000) 58
Wilson, M., see Domene, C. 333 (2001) 403
Wilson, P.J. and D.J. Tozer, NMR shielding constants from ab initio and Kohn–Sham electron densities 337 (2001) 341
Wimperis, S., see Ashbrook, S.E. 340 (2001) 500

Wine, P.H., see Estupiñán, E.G. 336 (2001) 109
Winiarczyk, P., see Rius i Riu, J. 333 (2001) 91
Winiarczyk, P., see Rius i Riu, J. 338 (2001) 285
Winkler, B., C.J. Pickard, V. Milman and G. Thimm, Systematic prediction of crystal structures 337 (2001) 36
Witkowska, B., see Iwanowski, R.J. 336 (2001) 226
Wojcik, M., see Baudin, M. 335 (2001) 517
Wolfers, P., see Tappero, R. 335 (2001) 449
Wolfrum, J., see Hanf, A. 340 (2001) 71
Wöll, Ch., K. Weiss and P.S. Bagus, Saturated hydrocarbons on a Cu surface: a new type of chemical interaction? 332 (2000) 553
Wolynec, P.P., see Wild, D.A. 332 (2000) 531
Wong, M.W., see Li, Z.-H. 337 (2001) 209
Wong, N., see Wang, X. 338 (2001) 367
Wong, N.B., see Liao, L.S. 333 (2001) 212
Wong, T.C., J. Kovac, C.S. Lee, L.S. Hung and S.T. Lee, Transient electroluminescence measurements on electron-mobility of *N*-arylbenzimidazoles 334 (2001) 61
Wong, W.K., see Meng, J.X. 332 (2000) 313
Wormer, P.E.S., see Rode, M. 334 (2001) 424
Woronowicz, E.A., see Weber, J.M. 339 (2001) 337
Worth, G.A. and L.S. Cederbaum, Mediation of ultrafast electron transfer in biological systems by conical intersections 338 (2001) 219
Wöste, L., see Socaciu, L.D. 340 (2001) 282
Wright, D., see Daly, G.M. 331 (2000) 47
Wright, J.C., see Murdoch, K.M. 335 (2001) 349
Wright, T.G. and E.P.F. Lee, The structure and stability of the complex formed between NO^+ and CO 340 (2001) 179
Wright, T.G., see Fleming, P.E. 332 (2000) 199
Wright, T.G., see Lee, E.P.F. 331 (2000) 533
Wright, T.G., see Lee, E.P.F. 336 (2001) 479
Wu, C.-X., Y. Yamazaki and O.-Y. Zhong-can, Anchoring-dependent phase separation in hexatic liquid crystals 338 (2001) 46
Wu, D., see Cao, A. 335 (2001) 150
Wu, G. and S. Dong, Orientations of the ^{17}O electric-field-gradient tensor and chemical shift tensor in benzamide: NMR of dipolar coupled spins 334 (2001) 265
Wu, G.T., see Chen, X.H. 336 (2001) 201
Wu, L.Z., see Lei, H. 333 (2001) 387
Wu, P., see Wang, P. 340 (2001) 261
Wu, X.C., W.H. Song, K.Y. Wang, T. Hu, B. Zhao, Y.P. Sun and J.J. Du, Preparation and photoluminescence properties of amorphous silica nanowires 336 (2001) 53

Xantheas, S.S., see Tzeli, D. 340 (2001) 538
Xi, F., see Wang, P. 340 (2001) 261
Xia, W.S., see Moskaleva, L.V. 331 (2000) 269
Xiang, L., Y.-G. Liu, A.-G. Jiang and D.-Y. Huang, Theoretical investigation of s-triazine derivatives as novel second-order nonlinear optical chromophores 338 (2001) 167
Xiao, F.R., see Wang, T.S. 334 (2001) 7
Xiao, S., see Shi, Z. 336 (2001) 19

Xie, D., Y. Lu and G. Yan, Theoretical studies for the potential energy surface and rovibrational spectra of Ne–HCN 339 (2001) 14
Xie, J., see Sun, M. 339 (2001) 413
Xie, S., see Liu, Y. 331 (2000) 31
Xie, S.S., see Sun, L.F. 336 (2001) 392
Xie, S.S., see Sun, L.F. 340 (2001) 222
Xin, H., see Zhong, S. 333 (2001) 133
Xin, J., see Su, H. 335 (2001) 17
Xin, X., see Song, Y. 338 (2001) 108
Xiong, Z.T., see Sun, L.F. 340 (2001) 222
Xu, C., see Cao, A. 335 (2001) 150
Xü, D., see Yang, P. 336 (2001) 76
Xu, G., see Jin, Z. 332 (2000) 461
Xu, G., see Jin, Z. 337 (2001) 43
Xu, G.Q., see Wang, Z.H. 338 (2001) 7
Xu, J.H., see Bernheim, R.A. 332 (2000) 1
Xu, L., see Fan, X.H. 334 (2001) 229
Xu, L., see Zhang, Z. 337 (2001) 18
Xu, Q.-H., Y.-Z. Ma and G.R. Fleming, Heterodyne detected transient grating spectroscopy in resonant and non-resonant systems using a simplified diffractive optics method 338 (2001) 254
Xu, Z., see Zeng, H. 338 (2001) 241

Yabushita, S., see Judai, K. 334 (2001) 277
Yagi, K., see Judai, K. 334 (2001) 277
Yamada, C., see Furuhashi, O. 337 (2001) 94
Yamaguchi, K., see Takano, Y. 335 (2001) 395
Yamaguchi, Y., N. Yasutake and M. Nagaoka, Theoretical prediction of proton chemical shift in supercritical water using gas-phase approximation 340 (2001) 129
Yamakata, A., T.-a. Ishibashi and H. Onishi, Time-resolved infrared absorption spectroscopy of photogenerated electrons in platinized TiO_2 particles 333 (2001) 271
Yamamoto, K., see Kubozono, Y. 335 (2001) 163
Yamano, T., see Tachikawa, H. 335 (2001) 305
Yamashita, H., see Furube, A. 336 (2001) 424
Yamazaki, I., see Kanada, T. 332 (2000) 442
Yamazaki, M., see Ohno, K. 332 (2000) 167
Yamazaki, Y., see Wu, C.-X. 338 (2001) 46
Yan, G., see Xie, D. 339 (2001) 14
Yan, Y., see Cheng, J. 333 (2001) 375
Yanagisawa, O., see He, J.L. 340 (2001) 431
Yang, C.L., see Cheng, J. 333 (2001) 375
Yang, H., see Bae, S.Y. 336 (2001) 219
Yang, H.D., see Chen, J.M. 337 (2001) 85
Yang, H.S., see Chen, X.H. 336 (2001) 201
Yang, P., M. I ü, D. Xü, D. Yuan and G. Zhou, Photoluminescence properties of ZnS nanoparticles co-doped with Pb^{2+} and Cu^{2+} 336 (2001) 76
Yang, S., see Cheng, J. 333 (2001) 375
Yang, S.-C., see White, J.D. 338 (2001) 263

Yang, S.X., see Li, W.Z. 335 (2001) 141
Yang, T., see Tsushima, S. 334 (2001) 365
Yang, T.-C., D.J. Sloop, S.I. Weissman and T.-S. Lin, Measurements of energy gap at the level anti-crossing region of the photo-excited triplet state of organic molecules 331 (2000) 489
Yang, X., see Peng, X. 340 (2001) 509
Yang, X., Z. Dai, A. Miura and N. Tamai, Different back electron transfer from titanium dioxide nanoparticles to tetra (4-sulfonatophenyl) porphyrin monomer and its J-aggregate 334 (2001) 257
Yang, Y., see Li, C. 340 (2001) 444
Yao, H. and K. Kimura, Large absorption reduction for mesoscopic thiacyanine J aggregates in solution 340 (2001) 211
Yao, J., see Shi, Z. 336 (2001) 19
Yasuike, T., see Judai, K. 334 (2001) 277
Yasutake, N., see Yamaguchi, Y. 340 (2001) 129
Yates Jr, J.T., see Lee, J.-G. 340 (2001) 21
Ye, C., see Wang, P. 340 (2001) 261
Ye, J., see Zou, Z. 332 (2000) 271
Ye, J., see Zou, Z. 333 (2001) 57
Yeh, C.-S., see Su, P.-H. 331 (2000) 420
Yin, J., see Sui, Y. 339 (2001) 186
Ying, L., M.I. Wallace and D. Klenerman, Two-state model of conformational fluctuation in a DNA hairpin-loop 334 (2001) 145
Yokojima, S., D. Zhou and G. Chen, Photoexcitations in poly(*p*-phenylenevinylene) aggregates 333 (2001) 397
Yoo, J.E., see Lee, C.J. 338 (2001) 113
Yoon, S.F., see Gan, B. 333 (2001) 23
Yoshida, N., M. Takechi, T. Asano, Y. Moroi, R. Humphry-Baker and M. Grätzel, Thermodynamics and kinetics of solubilization of naphthalene into anionic micelles 332 (2000) 265
Yoshiki Franzén, K., see Rius i Riu, J. 333 (2001) 91
Yoshiki Franzén, K., see Rius i Riu, J. 338 (2001) 285
Yoshioka, Y., see Takano, Y. 335 (2001) 395
Yu, D.L., see He, J.L. 340 (2001) 431
Yu, D.L., see Wang, T.S. 334 (2001) 7
Yu, G., D. Shen, Y. Liu and D. Zhu,
Yu. G., D. Shen, Y. Liu and D. Zhu Fluorescence stability of 8-hydroxyquinoline aluminum 333 (2001) 207
Yu, H.G. and A.J.C. Varandas, Ab initio theoretical calculation and potential energy surface for ground-state HO_3 334 (2001) 173
Yu, H.-G., Quantum dynamics of the reaction of hydrogen atom with methane 332 (2000) 538
Yu, J., see Gan, B. 333 (2001) 23
Yu, S., see Zhou, X. 339 (2001) 117
Yu, W.-S., see Chou, P.-T. 340 (2001) 89
Yu, Y., see Ding, C.-F. 331 (2000) 163
Yuan, D., see Yang, P. 336 (2001) 76
Yuan, J., see Meng, J.X. 332 (2000) 313

Yuan, L., K. Saito, C. Pan, F.A. Williams and A.S. Gordon, Nanotubes from methane flames 340 (2001) 237
Yuan, L.-F., see Lin, H. 332 (2000) 569
Yuan, Z. and W. Zhou, A novel morphology of mesoporous molecular sieve MCM-41 333 (2001) 427
Yudasaka, M., see Bandow, S. 337 (2001) 48
Yudasaka, M., see Kasuya, D. 337 (2001) 25
Yudasaka, M., see Kokai, F. 332 (2000) 449
Yudasaka, M., see Murata, K. 331 (2000) 14
Yudasaka, M., see Zhang, M. 336 (2001) 196
Yujing, M. and A. Mellouki, Temperature dependence for the rate constants of the reaction of OH radicals with selected alcohols 333 (2001) 63
Yuxiao, W., see Song, Y. 338 (2001) 108

Zaera, F. and C.S. Gopinath, Evidence for an N_2O intermediate in the catalytic reduction of NO to N_2 on rhodium surfaces 332 (2000) 209
Zahn, D. and J. Brickmann, A comparative study of proton migration in water and deuteron transport in heavy water by means of mixed quantum/classical molecular dynamics simulation 331 (2000) 224
Zahn, G., see Spichiger, D. 337 (2001) 391
Zalyubovsky, S.J., D. Wang and T.A. Miller, Observation of the $\tilde{A}$–$\tilde{X}$ electronic transition of the CF_3O_2 radical 335 (2001) 298
Zamora, M.A., see Torday, L.L. 334 (2001) 381
Zannoni, C., see Bacchiocchi, C. 336 (2001) 253
Zannoni, C., see Burnell, E.E. 331 (2000) 455
Zasetsky, A.Yu. and I.M. Svishchev, Local order in liquid oxygen: computer simulations with point charge model 334 (2001) 107
Zavelani-Rossi, M., see Cerullo, G. 335 (2001) 27
Zell, C.A. and W. Freyland, In situ STM and STS study of $Ni_x Al_{1-x}$ alloy formation on Au(111) by electrodeposition from a molten salt electrolyte 337 (2001) 293
Zeng, H., C. Liu, S. Tokura, M. Kira and Y. Segawa, Optical limiting and bistability of a σ–π photoconductive copolymer 331 (2000) 71
Zeng, H., Z. Sun, Y. Segawa, F. Lin, S. Mao and Z. Xu, Conductivity of fullerene-doped optical glasses 338 (2001) 241
Zeppenfeld, P., see Lehner, B. 336 (2001) 123
Zerza, G., see Brabec, C.J. 340 (2001) 232
Zgierski, M.Z., see Andruniow, T. 331 (2000) 502
Zgierski, M.Z., see Andruniow, T. 331 (2000) 509
Zgierski, M.Z., see Siebrand, W. 334 (2001) 127
Zhang, B., L.-E. Berg and T. Hansson, "Wavepacket dynamics and predissociation of the D $^1\Pi_u$ state of Rb_2" [Chem. Phys. Lett. 325 (2000) 577] 339 (2001) 438
Zhang, C., see Sun, M. 339 (2001) 413
Zhang, D., see Hu, H. 340 (2001) 370
Zhang, F., Z. Li and L. Wang, Hexagonal chains with maximal total π -electron energy 337 (2001) 131
Zhang, F., Z. Li and L. Wang, Hexagonal chains with minimal total π-electron energy 337 (2001) 125
Zhang, J., see Liu, Y. 331 (2000) 31

Zhang, J., see Zheng, M. 334 (2001) 298
Zhang, J.-P., T. Inaba, Y. Watanabe and Y. Koyama, Sub-picosecond time-resolved absorption spectroscopy of all-*trans*-neurosporene in solution and bound to the LH2 complex from *Rhodobacter sphaeroides* G1C 331 (2000) 154
Zhang, J.-P., T. Inaba, Y. Watanabe and Y. Koyama, Excited-state dynamics among the $1B_u^+$, $1B_u^-$ and $2A_g^-$ states of all-*trans*-neurosporene as revealed by near-infrared time-resolved absorption spectroscopy 332 (2000) 351
Zhang, J.-P., T. Inaba, Y. Watanabe and Y. Koyama, Partition of carotenoid-to-bacteriochlorophyll singlet-energy transfer through two channels in the LH2 complex from *Rhodobacter sphaeroides* G1C 340 (2001) 484
Zhang, K.-C., L. Liu, T.-W. Mu and Q.-X. Guo, Ab initio calculations on the inclusion complexation of cyclobis(paraquat-*p*-phenylene) 333 (2001) 195
Zhang, K.-C., see Chen, R. 338 (2001) 61
Zhang, L., J. Dong and M. Zhou, Formation and characterization of the AsCO and $AsCO^-$ molecules. A matrix isolation FTIR and theoretical study 335 (2001) 334
Zhang, L., see Varandas, A.J.C. 331 (2000) 474
Zhang, L., see Varandas, A.J.C. 340 (2001) 62
Zhang, L., see Zheng, M. 334 (2001) 298
Zhang, L., see Zhou, X. 339 (2001) 117
Zhang, L.D., see Lei, Y. 338 (2001) 231
Zhang, L.D., see Wang, Y.W. 339 (2001) 174
Zhang, L.L., see Meng, J.X. 332 (2000) 313
Zhang, L.-M., see Clark, J. 340 (2001) 45
Zhang, M., M. Yudasaka and S. Iijima, Single-wall carbon nanotubes: a high yield of tubes through laser ablation of a crude-tube target 336 (2001) 196
Zhang, Q., see Gan, B. 333 (2001) 23
Zhang, Q., see Song, Y. 338 (2001) 108
Zhang, Q.-y., see Qu, Z.-w. 336 (2001) 325
Zhang, Q.-y., see Qu, Z.-w. 339 (2001) 140
Zhang, R.Q., see Zhou, X.T. 332 (2000) 215
Zhang, S., L. Gan and C. Huang, Photoelectric response of pyrrolidinofullerene and bis-pyrrolidinofullerene LB films 331 (2000) 143
Zhang, S., see Wang, P. 340 (2001) 261
Zhang, X., see Lu, J. 332 (2000) 219
Zhang, X., see Lu, J. 332 (2000) 51
Zhang, X., see Zheng, M. 334 (2001) 298
Zhang, X.B., see Chen, X.H. 336 (2001) 201
Zhang, X.-B., see Gan, B. 333 (2001) 23
Zhang, X.X., Z.Q. Li, G.H. Wen, K.K. Fung, J. Chen and Y. Li, Microstructure and growth of bamboo-shaped carbon nanotubes 333 (2001) 509
Zhang, Y., N.W. Franklin, R.J. Chen and H. Dai, Metal coating on suspended carbon nanotubes and its implication to metal–tube interaction 331 (2000) 35
Zhang, Z., X.H. Fan, L. Xu, C.S. Lee and S.T. Lee, Morphology and growth mechanism study of self-assembled silicon nanowires synthesized by thermal evaporation 337 (2001) 18
Zhao, B., see Wu, X.C. 336 (2001) 53
Zhao, L., see Waldmann, O. 332 (2000) 73

Zhao, W., see Murdoch, K.M. 335 (2001) 349
Zhao, X., see Lu, J. 332 (2000) 219
Zhao, X., see Lu, J. 332 (2000) 51
Zheng, J.C., see Guo, Y.P. 339 (2001) 319
Zheng, J.P., see Ma, Z. 331 (2000) 64
Zheng, M., L. Zhang, X. Zhang, J. Zhang and G. Li, Fabrication and optical absorption of ordered indium oxide nanowire arrays embedded in anodic alumina membranes 334 (2001) 298
Zheng, Y.F., see Fan, X.H. 334 (2001) 229
Zhong, J., see Chen, Z. 333 (2001) 126
Zhong, J., see Chen, Z. 333 (2001) 96
Zhong, J., see Lin, G. 335 (2001) 249
Zhong, S. and H. Xin, Effects of colored noise on internal stochastic resonance in a chemical model system 333 (2001) 133
Zhong, Z.Y., see Sun, L.F. 340 (2001) 222
Zhong-can, O.-Y., see Wu, C.-X. 338 (2001) 46
Zhou, D., see Yokojima, S. 333 (2001) 397
Zhou, G., see Yang, P. 336 (2001) 76
Zhou, G., W. Duan and B. Gu, First-principles study on morphology and mechanical properties of single-walled carbon nanotube 333 (2001) 344
Zhou, G.Y., see Lei, H. 333 (2001) 387
Zhou, M., see Zhang, L. 335 (2001) 334
Zhou, W., see Yuan, Z. 333 (2001) 427
Zhou, W.Y., see Sun, L.F. 336 (2001) 392
Zhou, W.Y., see Sun, L.F. 340 (2001) 222
Zhou, X., S. Yu, J. Li, Z. Sheng, L. Zhang and X. Ma, Ab initio calculations of the potential energy surface for the reaction $N(^2D) + CH_3F$ 339 (2001) 117
Zhou, X.T., R.Q. Zhang, H.Y. Peng, N.G. Shang, N. Wang, I. Bello, C.S. Lee and S.T. Lee, Highly efficient and stable photoluminescence from silicon nanowires coated with SiC 332 (2000) 215
Zhu, D., see Li, Y. 337 (2001) 403
Zhu, D., see Liu, Y. 331 (2000) 31
Zhu, D., see Shi, Z. 336 (2001) 19
Zhu, D., see Wang, X. 339 (2001) 36
Zhu, D., see Wang, X. 340 (2001) 419
Zhu, D., see Yu, G. 333 (2001) 207
Zhu, H., see Qu, Z.-w. 336 (2001) 325
Zhu, H., see Qu, Z.-w. 339 (2001) 140
Zhu, X., see Peng, X. 340 (2001) 509
Zhu, X., see Wang, J. 340 (2001) 98
Zhu, Z.-k., see Sui, Y. 339 (2001) 186
Zigmantas, D., see Theander, M. 337 (2001) 277
Zou, B.S., see Volkov, V.V. 337 (2001) 117
Zou, G.T., see He, J.L. 340 (2001) 431
Zou, S., S. Skokov and J.M. Bowman, Ab initio calculation of resonance energies and widths of HOCl($7\nu_{OH}$ and $8\nu_{OH}$) and comparison with experiment 339 (2001) 290
Zou, X.P., see Sun, L.F. 336 (2001) 392

Zou, X.P., see Sun, L.F. 340 (2001) 222
Zou, Z., J. Ye and H. Arakawa, Photocatalytic and photophysical properties of a novel series of solid photocatalysts, Bi_2MNbO_7 ($M = Al^{3+}$, Ga^{3+} and In^{3+}) 333 (2001) 57
Zou, Z., J. Ye and H. Arakawa, Structural properties of $InNbO_4$ and $InTaO_4$: correlation with photocatalytic and photophysical properties 332 (2000) 271
Zubek, M., see Olszewski, R. 340 (2001) 249
Zumofen, G., see Segura, J.-M. 340 (2001) 77
Zych, E., see Dereń, P.J. 332 (2000) 308

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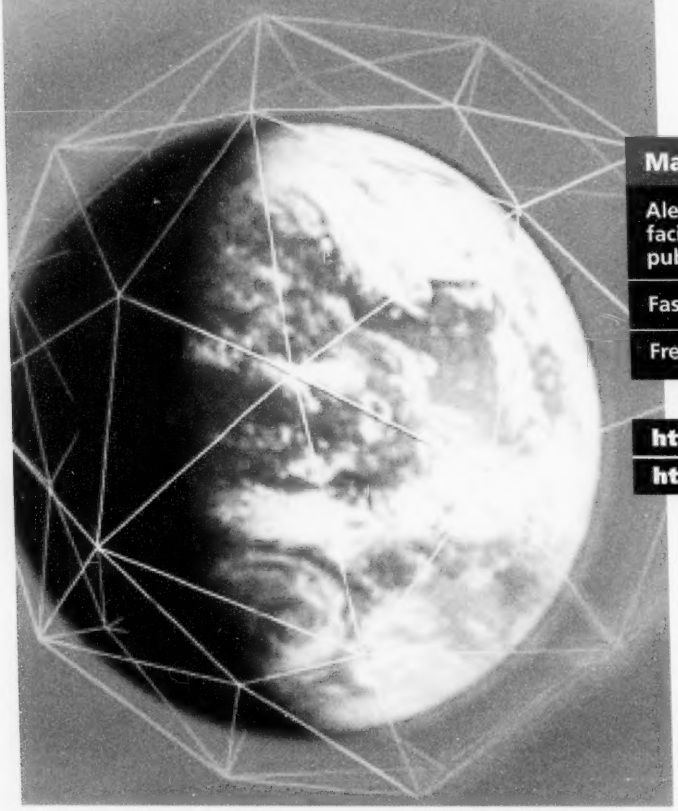

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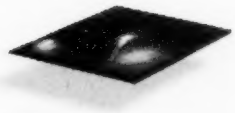

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